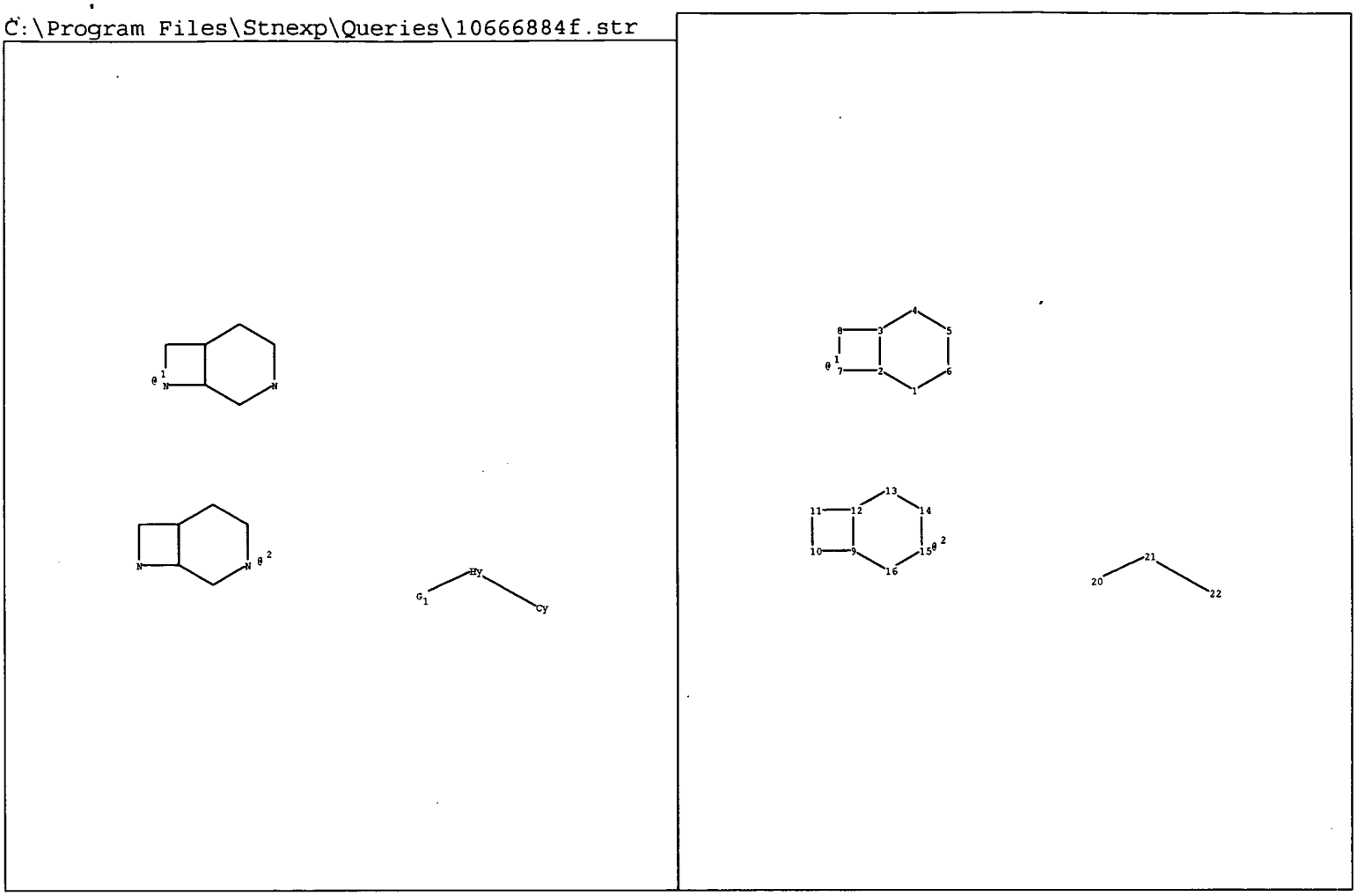
10666884

```
    FILE 'REGISTRY' ENTERED AT 12:57:32 ON 29 APR 2005
L1                STRUCTURE UPLOADED
L2              0 S L1
L3              5 S L1 SSS FULL

     FILE 'CAPLUS' ENTERED AT 12:58:28 ON 29 APR 2005
L4              1 S L3

     FILE 'MARPAT' ENTERED AT 12:59:11 ON 29 APR 2005
L5              0 S L3
L6              1 S L3 SSS FULL

     FILE 'CAPLUS' ENTERED AT 12:59:40 ON 29 APR 2005
L7              1 S L6 NOT L4

     FILE 'REGISTRY' ENTERED AT 13:08:57 ON 29 APR 2005
                E 848591-72-0/RN
L8              1 S E3
L9             83 S 191.188/RID

     FILE 'CAPLUS' ENTERED AT 13:11:17 ON 29 APR 2005
L10             6 S L9

=> s l10 not l4
L11             5 L10 NOT L4
```

C:\Program Files\Stnexp\Queries\10666884f.str



chain nodes :
20 21 22
ring nodes :
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16
chain bonds :
20-21 21-22
ring bonds :
1-2 1-6 2-3 2-7 3-4 3-8 4-5 5-6 7-8 9-10 9-12 9-16 10-11 11-12 12-13 13-14
14-15 15-16
exact/norm bonds :
14-15 20-21 21-22
exact bonds :
1-2 1-6 2-3 2-7 3-4 3-8 4-5 5-6 7-8 9-10 9-12 9-16 10-11 11-12 12-13 13-14
15-16

G1:[*1],[*2]

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom
12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 20:CLASS 21:Atom 22:Atom
Generic attributes :
21:
Saturation : Unsaturated
Number of Carbon Atoms : less than 7
Type of Ring System : Monocyclic

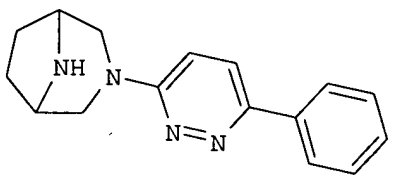
10666884

L4 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2005 ACS on STN
AN 2005:259679 CAPLUS
DN 142:336373
TI A preparation of diazabicycloakane derivatives, useful as modulators of α7 nicotinic acetylcholine receptors
IN Basha, Anwer; Bunnelle, William H.; Dart, Michael J.; Gallagher, Megan E.; Ji, Jianguo; Li, Tao; Pace, Jennifer M.; Ryther, Keith B.; Tietje, Karin R.
PA USA
SO U.S. Pat. Appl. Publ., 47 pp.
CODEN: USXXCO
DT Patent
LA English
FAN.CNT 1

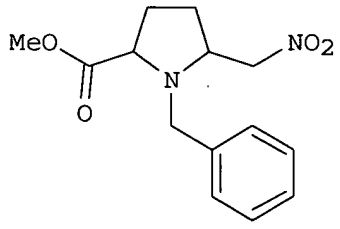
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI US 2005065178	A1	20050324	US 2003-666884	20030919
WO 2005028477	A1	20050331	WO 2004-US30735	20040917

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

PRAI US 2003-666884 A 20030919
GI



I



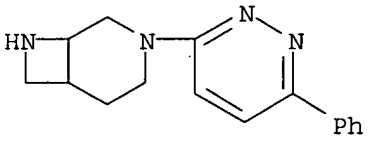
II

AB The invention relates to a preparation of diazabicycloakane derivs. of formula

Z-Ar1-Ar2 [wherein: Z is a diazabicyclic amine; Ar1 is a 5- or 6-membered (hetero)aromatic ring; and Ar2 is selected from (un)substituted 5-membered heteroaryl ring, 6-membered heteroaryl ring, or 3,4-(methylenedioxy)phenyl, etc.], useful as modulators of α7 nicotinic acetylcholine receptors (nAChRs). The invention compds. are useful for the treatment of Alzheimer's disease, Pick's disease, AIDS dementia, and attention deficit, etc. For instance, pyridazinyldiazabicyclooctane derivative I•(p-MeC6H4SO3H)2 was prepared via heterocyclization of pyrrolidine derivative II and 7 subsequent steps (a yield of the heterocyclization step was 36%). The invention compds. had Ki values of from about 1 nM to about 10 μM.

IT **848591-72-0P 848591-82-2P 848591-83-3P 848591-84-4P**
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of diazabicycloakane derivs. useful as modulators of α7 nicotinic acetylcholine receptors)

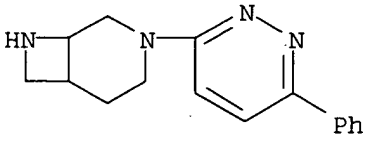
RN 848591-72-0 CAPLUS
CN 3,8-Diazabicyclo[4.2.0]octane, 3-(6-phenyl-3-pyridazinyl)- (9CI) (CA INDEX NAME)



RN 848591-82-2 CAPLUS
CN 3,8-Diazabicyclo[4.2.0]octane, 3-(6-phenyl-3-pyridazinyl)-, bis(trifluoroacetate) (9CI) (CA INDEX NAME)

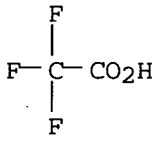
CM 1

CRN 848591-72-0
CMF C16 H18 N4

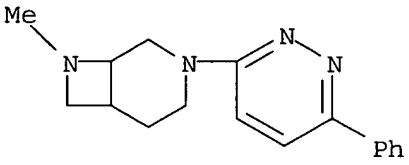


CM 2

CRN 76-05-1
CMF C2 H F3 O2



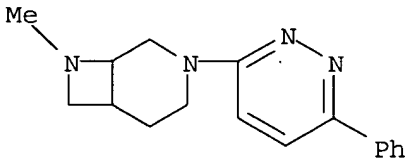
RN 848591-83-3 CAPLUS
CN 3,8-Diazabicyclo[4.2.0]octane, 8-methyl-3-(6-phenyl-3-pyridazinyl)- (9CI) (CA INDEX NAME)



RN 848591-84-4 CAPLUS
CN 3,8-Diazabicyclo[4.2.0]octane, 8-methyl-3-(6-phenyl-3-pyridazinyl)-, bis(4-methylbenzenesulfonate) (9CI) (CA INDEX NAME)

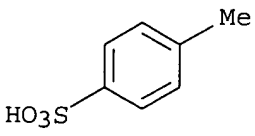
CM 1

CRN 848591-83-3
CMF C17 H20 N4



CM 2

CRN 104-15-4
CMF C7 H8 O3 S

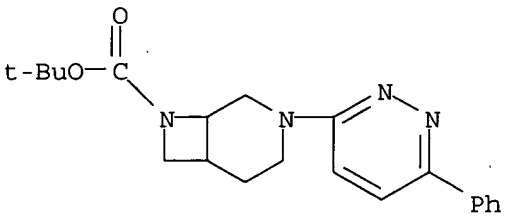


IT **848591-81-1P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT

(Reactant or reagent)
(preparation of diazabicycloakane derivs. useful as modulators of α7 nicotinic acetylcholine receptors)

RN 848591-81-1 CAPLUS

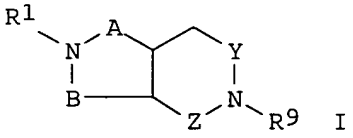
CN 3,8-Diazabicyclo[4.2.0]octane-8-carboxylic acid, 3-(6-phenyl-3-pyridazinyl)-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



L7 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2005 ACS on STN
AN 2001:798225 CAPLUS
DN **135:344471**
TI Preparation of diazabicyclic compounds as central nervous system active agents
IN Schrimpf, Michael R.; Tietje, Karin R.; Toupence, Richard B.; Ji, Jianguo; Basha, Anwer; Bunnelle, William H.; Daanen, Jerome F.; Pace, Jennifer M.; Sippy, Kevin B.
PA Abbott Laboratories, USA
SO PCT Int. Appl., 190 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2001081347	A2	20011101	WO 2001-US13798	20010427
	WO 2001081347	A3	20020131		
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
	RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
	US 2002019388	A1	20020214	US 2001-833914	20010412
	US 6809105	B2	20041026		
	CA 2407094	AA	20011101	CA 2001-2407094	20010427
	BR 2001007246	A	20021001	BR 2001-7246	20010427
	EP 1284976	A2	20030226	EP 2001-944118	20010427
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
	JP 2003531210	T2	20031021	JP 2001-578437	20010427
	NZ 521734	A	20041029	NZ 2001-521734	20010427
	ZA 2002008274	A	20040211	ZA 2002-8274	20021014
	NO 2002005107	A	20021219	NO 2002-5107	20021024
	BG 107303	A	20030731	BG 2002-107303	20021121
	US 2004186107	A1	20040923	US 2004-810999	20040326
PRAI	US 2000-200111P	P	20000427		
	US 2000-559943	A	20000427		
	US 2001-833914	A	20010412		
	WO 2001-US13798	W	20010427		

OS MARPAT 135:344471
GI



I

AB Diazabicyclic compds. (I; e.g. cis-2-(3-pyridinyl)octahydropyrrolo[3,4-

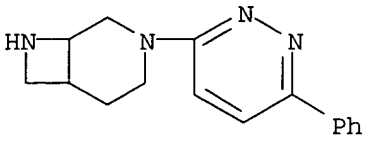
c]pyrrole dihydrochloride), pharmaceutical compns. of these compds., and use of said compns. to control synaptic transmission in mammals are claimed. In I: A = covalent bond, CH2, CH2CH2, and CH2CH2CH2; B = CH2 and CH2CH2, provided that when A is CH2CH2CH2, then B is CH2; Y = covalent bond, CH2, and CH2CH2; Z = covalent bond, CH2, and CH2CH2, provided that when Y is CH2CH2, then Z is a covalent bond and further provided that when Z is CH2CH2, then Y is a covalent bond. R1 = optionally substituted phthalazin-1-yl, pyridin-3-yl, pyrazinyl, pyrimidin-5-yl, pyridazin-3-yl, quinolin-3-yl, thieno[3,2-b]pyridin-2-yl, furano[3,2-b]pyridin-2-yl, thieno[3,2-b]pyridin-3-yl, furano[3,2-b]pyridin-3-yl, furano[3,2-b]pyridin-6-yl, thieno[3,2-b]pyridin-6-yl, furano[2,3-b]pyridin-5-yl, thieno[2,3-b]pyridin-5-yl, isothiazol-5-yl, isoxazol-5-yl. R9 = H, alkoxycarbonyl, alkyl, amino, aminoalkyl, aminocarbonylalkyl, benzyloxycarbonyl, cyanoalkyl, dihydro-3-pyridinylcarbonyl, hydroxy, hydroxyalkyl, and phenoxycarbonyl. Values are reported for nicotinic acetylcholine receptor binding potencies and effectiveness of nicotinic acetylcholine receptor ligands as analgesic agents and in the formalin test for some of the claimed compds. Ninety-six example prepns. are given but the methods of preparation are not claimed. The crystal and mol. structures of (3aS,6aS)-5-[(4-nitrophenyl)sulfonyl]-1-((1R)-1-phenylethyl)octahydropyrrolo[3,4-b]pyrrole and tert-Bu (3S,4S)-4-(hydroxymethyl)-3-[((1S)-1-phenylethyl)amino]-1-piperidinecarboxylate were determined by x-ray crystallog.

10666884

RN **848591-72-0** REGISTRY
ED Entered STN: 15 Apr 2005
CN 3,8-Diazabicyclo[4.2.0]octane, 3-(6-phenyl-3-pyridazinyl)- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C16 H18 N4
CI COM
SR CA
LC STN Files: CA, CAPLUS
DT.CA CAplus document type: Patent
RL.P Roles from patents: BIOL (Biological study); PREP (Preparation); USES (Uses)

Ring System Data

Elemental Analysis EA	Elemental Sequence ES	Size of the Rings SZ	Ring System Formula RF	Ring Identifier RID	RID Occurrence Count
C6	C6	6	C6	46.150.18	1
C4N2	N2C4	6	C4N2	46.169.19	1
C3N-C5N	NC3-NC5	4-6	C6N2	191.188.2	1



Predicted Properties (PPROP)

PROPERTY (CODE)	VALUE	CONDITION	NOTE
Bioconc. Factor (BCF)	1	pH 1	(1) ACD
Bioconc. Factor (BCF)	1	pH 4	(1) ACD
Bioconc. Factor (BCF)	1	pH 7	(1) ACD
Bioconc. Factor (BCF)	1	pH 8	(1) ACD
Bioconc. Factor (BCF)	1.48	pH 10	(1) ACD
Boiling Point (BP)	521.0+/-40.0 deg C	760 Torr	(1) ACD
Enthalpy of Vap. (HVAP)	79.41+/-3.0 kJ/mol		(1) ACD
Flash Point (FP)	268.9+/-49.2 deg C		(1) ACD
Freely Rotatable Bonds (FRB)	2		(1) ACD
H acceptors (HAC)	4		(1) ACD
H donors (HD)	1		(1) ACD
Koc (KOC)	1	pH 1	(1) ACD
Koc (KOC)	1	pH 4	(1) ACD
Koc (KOC)	1	pH 7	(1) ACD
Koc (KOC)	1	pH 8	(1) ACD
Koc (KOC)	31.1	pH 10	(1) ACD
logD (LOGD)	-3.68	pH 1	(1) ACD

logD (LOGD)	-3.61	pH 4	(1) ACD
logD (LOGD)	-1.78	pH 7	(1) ACD
logD (LOGD)	-1.08	pH 8	(1) ACD
logD (LOGD)	0.72	pH 10	(1) ACD
logP (LOGP)	1.322+/-0.516		(1) ACD
Molar Solubility (SLB.MOL)	>=1 mol/L	pH 1	(1) ACD
Molar Solubility (SLB.MOL)	>=1 mol/L	pH 4	(1) ACD
Molar Solubility (SLB.MOL)	>=1 mol/L	pH 7	(1) ACD
Molar Solubility (SLB.MOL)	>=0.1 - <1 mol/L	pH 8	(1) ACD
Molar Solubility (SLB.MOL)	>=0.01 - <0.1 mol/L	pH 10	(1) ACD
Molecular Weight (MW)	266.34		(1) ACD
pKa (PKA)	10.48+/-0.40	Most Basic	(1) ACD
Vapor Pressure (VP)	5.93E-11 Torr	25 deg C	(1) ACD

(1) Calculated using Advanced Chemistry Development (ACD/Labs) Software Solaris V4.76 ((C) 1994-2005 ACD/Labs)

See HELP PROPERTIES for information about property data sources in REGISTRY.

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

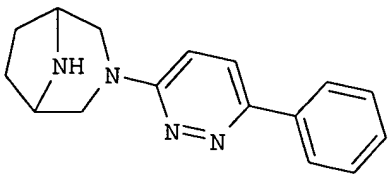
REFERENCE 1

AN 142:336373 CA
TI A preparation of diazabicycloakane derivatives, useful as modulators of α7 nicotinic acetylcholine receptors
IN Basha, Anwer; Bunnelle, William H.; Dart, Michael J.; Gallagher, Megan E.; Ji, Jianguo; Li, Tao; Pace, Jennifer M.; Ryther, Keith B.; Tietje, Karin R.
PA USA
SO U.S. Pat. Appl. Publ., 47 pp.
CODEN: USXXCO
DT Patent
LA English
IC ICM C07D471-02
ICS A61K031-4745
NCL 514300000
CC 28-15 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 1, 63
FAN.CNT 1

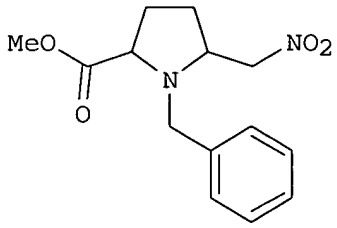
	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 2005065178	A1	20050324	US 2003-666884	20030919
	WO 2005028477	A1	20050331	WO 2004-US30735	20040917

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

PRAI US 2003-666884 20030919
GI



I



II

AB The invention relates to a preparation of diazabicycloakane derivs. of formula Z-Ar1-Ar2 [wherein: Z is a diazabicyclic amine; Ar1 is a 5- or 6-membered (hetero)aromatic ring; and Ar2 is selected from (un)substituted 5-membered heteroaryl ring, 6-membered heteroaryl ring, or 3,4-(methylenedioxy)phenyl, etc.], useful as modulators of α7 nicotinic acetylcholine receptors (nAChRs). The invention compds. are useful for the treatment of Alzheimer's disease, Pick's disease, AIDS dementia, and attention deficit, etc. For instance, pyridazinyldiazabicyclooctane derivative I•(p-MeC6H4SO3H)2 was prepared via heterocyclization of pyrrolidine derivative II and 7 subsequent steps (a yield of the heterocyclization step was 36%). The invention compds. had Ki values of from about 1 nM to about 10 μM.

ST diazabicycloakane prepn modulator 7 alpha nicotinic acetylcholine receptor antialzheimer

IT AIDS (disease)
(AIDS dementia complex, treatment of; preparation of diazabicycloakane derivs. useful as modulators of α7 nicotinic acetylcholine receptors)

IT Mental disorder
(AIDS dementia, treatment of; preparation of diazabicycloakane derivs. useful as modulators of α7 nicotinic acetylcholine receptors)

IT Mental disorder
(Pick's disease, treatment of; preparation of diazabicycloakane derivs. useful as modulators of α7 nicotinic acetylcholine receptors)

IT Mental disorder
(attention deficit hyperactivity disorder, treatment of; preparation of diazabicycloakane derivs. useful as modulators of α7 nicotinic acetylcholine receptors)

IT Mental disorder
(cognitive, mild, treatment of; preparation of diazabicycloakane derivs. useful as modulators of α7 nicotinic acetylcholine receptors)

IT Nerve, disease

(degeneration, treatment of; preparation of diazabicycloakane derivs. useful as modulators of α7 nicotinic acetylcholine receptors)

IT Cognition
(disorder, mild, treatment of; preparation of diazabicycloakane derivs. useful as modulators of α7 nicotinic acetylcholine receptors)

IT Anti-Alzheimer's agents
Antipsychotics
(preparation of diazabicycloakane derivs. useful as modulators of α7 nicotinic acetylcholine receptors)

IT Mental disorder
(senile psychosis, treatment of; preparation of diazabicycloakane derivs. useful as modulators of α7 nicotinic acetylcholine receptors)

IT Alzheimer's disease
Schizophrenia
(treatment of; preparation of diazabicycloakane derivs. useful as modulators of α7 nicotinic acetylcholine receptors)

IT Nicotinic receptors
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(α7; preparation of diazabicycloakane derivs. useful as modulators of α7 nicotinic acetylcholine receptors)

IT 848591-93-5P 848592-03-0P 848592-09-6P 848592-58-5P
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation of diazabicycloakane derivs. useful as modulators of α7 nicotinic acetylcholine receptors)

IT 848591-60-6P 848591-61-7P 848591-64-0P 848591-66-2P 848591-71-9P
848591-72-0P 848591-82-2P 848591-83-3P 848591-84-4P 848591-85-5P
848591-88-8P 848591-89-9P 848591-90-2P 848591-91-3P 848591-94-6P
848591-95-7P 848591-96-8P 848591-98-0P 848591-99-1P 848592-04-1P
848592-05-2P 848592-06-3P 848592-10-9P 848592-11-0P 848592-12-1P
848592-14-3P 848592-15-4P 848592-17-6P 848592-18-7P 848592-19-8P
848592-20-1P 848592-22-3P 848592-23-4P 848592-24-5P 848592-25-6P
848592-27-8P 848592-28-9P 848592-29-0P 848592-30-3P 848592-34-7P
848592-35-8P 848592-37-0P 848592-42-7P 848592-43-8P 848592-44-9P
848592-46-1P 848592-47-2P 848592-49-4P 848592-50-7P 848592-51-8P
848592-52-9P 848592-54-1P 848592-55-2P 848592-59-6P 848592-60-9P
848592-62-1P 848592-68-7P 848592-71-2P 848592-91-6P 848592-93-8P
848592-95-0P 848592-98-3P 848593-07-7P 848593-10-2P 848593-13-5P
848593-15-7P 848593-22-6P 848593-24-8P 848593-26-0P 848593-28-2P
848593-36-2P 848593-38-4P 848593-40-8P 848593-42-0P 848593-48-6P
848593-50-0P 848593-52-2P 848593-54-4P 848593-75-9P 848593-77-1P
848593-83-9P 848593-85-1P 848593-87-3P 848593-89-5P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of diazabicycloakane derivs. useful as modulators of α7 nicotinic acetylcholine receptors)

IT 100-46-9, Benzenemethanamine, reactions 116-11-0, 2-Methoxypropene 141-30-0, 3,6-Dichloropyridazine 149-87-1 501-53-1, Benzyl chloroformate 541-59-3, Maleimide 542-92-7, Cyclopentadiene, reactions 626-55-1, 3-Bromopyridine 1126-00-7, 1-Phenylpyrazole 1423-26-3, 3-(Trifluoromethyl)phenylboronic acid 2002-03-1 2398-37-0, 3-Bromoanisole 3356-89-6 3886-69-9 4175-78-4, 2,5-Dibromothiazole 4595-59-9, 5-Bromopyrimidine 5122-95-2, 3-Biphenylboronic acid 5720-07-0, p-Methoxyphenylboronic acid 6542-88-7, Aminoacetaldehyde 10365-98-7, m-Methoxyphenylboronic acid 17136-36-6, (Benzylamino)acetic acid 17933-03-8, m-Tolylboronic acid 20375-65-9 24255-23-0 30418-59-8,

3-Aminobenzeneboronic acid 52763-21-0 53939-30-3,
5-Bromo-2-chloropyridine 55552-70-0, 3-Furylboronic acid 93102-05-7
94839-07-3 98437-23-1 165893-95-8
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of diazabicycloakane derivs. useful as modulators of α7 nicotinic acetylcholine receptors)

IT 15115-52-3P 53645-95-7P 71233-25-5P 86732-28-7P 86755-80-8P
93428-56-9P 103301-78-6P 114790-39-5P 141449-85-6P 149771-44-8P
186202-73-3P 188345-71-3P 194032-49-0P 246510-69-0P 246510-70-3P
252770-09-5P 370880-75-4P 370880-76-5P 370881-68-8P 370882-67-0P
569682-60-6P 799279-81-5P 799279-83-7P 824982-17-4P 824982-18-5P
824982-19-6P 848591-62-8P 848591-63-9P 848591-65-1P 848591-67-3P,
2,4-Diformylpyrrolidine-1-carboxylic acid tert-butyl ester 848591-68-4P
848591-69-5P 848591-70-8P 848591-73-1P 848591-74-2P 848591-75-3P
848591-76-4P 848591-77-5P 848591-78-6P 848591-79-7P 848591-80-0P
848591-81-1P 848591-86-6P 848591-87-7P 848591-92-4P 848591-97-9P
848592-00-7P 848592-01-8P 848592-02-9P 848592-07-4P 848592-08-5P
848592-13-2P 848592-16-5P 848592-21-2P 848592-26-7P 848592-31-4P
848592-32-5P 848592-33-6P 848592-36-9P 848592-38-1P 848592-39-2P
848592-40-5P 848592-41-6P 848592-45-0P 848592-48-3P 848592-53-0P
848592-56-3P 848592-57-4P 848592-79-0P 848592-84-7P 848592-86-9P
848592-88-1P 848593-00-0P 848593-18-0P 848593-20-4P 848593-30-6P
848593-33-9P 848593-46-4P 848593-56-6P 848593-58-8P 848593-60-2P
848593-62-4P 848593-64-6P 848593-66-8P 848593-68-0P 848593-70-4P
848593-73-7P 848593-79-3P 848593-81-7P 848593-91-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of diazabicycloakane derivs. useful as modulators of α7 nicotinic acetylcholine receptors)

10666884

```
=> d his

     (FILE 'HOME' ENTERED AT 12:57:23 ON 29 APR 2005)

     FILE 'REGISTRY' ENTERED AT 12:57:32 ON 29 APR 2005
L1             STRUCTURE UPLOADED
L2           0 S L1
L3           5 S L1 SSS FULL

     FILE 'CAPLUS' ENTERED AT 12:58:28 ON 29 APR 2005
L4           1 S L3

     FILE 'MARPAT' ENTERED AT 12:59:11 ON 29 APR 2005
L5           0 S L3
L6           1 S L3 SSS FULL

     FILE 'CAPLUS' ENTERED AT 12:59:40 ON 29 APR 2005
L7           1 S L6 NOT L4

     FILE 'REGISTRY' ENTERED AT 13:08:57 ON 29 APR 2005
               E 848591-72-0/RN
L8           1 S E3
L9          83 S 191.188/RID

     FILE 'CAPLUS' ENTERED AT 13:11:17 ON 29 APR 2005
L10          6 S L9

=> s l10 not l4
L11          5 L10 NOT L4

=> d 1-5 bib abs hitstr

L11  ANSWER 1 OF 5  CAPLUS  COPYRIGHT 2005 ACS on STN
AN   2002:675469  CAPLUS
DN   137:337697
TI   Efficient Entry to Highly Functionalized β-Lactams by Regio- and
     Stereoselective 1,3-Dipolar Cycloaddition Reaction of 2-Azetidinone-
     Tethered Nitrones. Synthetic Applications
AU   Alcaide, Benito; Almendros, Pedro; Alonso, Jose M.; Aly, Moustafa F.;
     Pardo, Carmen; Saez, Elena; Torres, M. Rosario
CS   Facultad de Quimica, Departamento de Quimica Organica I, Universidad
     Complutense, Madrid, 28040, Spain
SO   Journal of Organic Chemistry (2002), 67(20), 7004-7013
     CODEN: JOCEAH; ISSN: 0022-3263
PB   American Chemical Society
DT   Journal
LA   English
OS   CASREACT 137:337697
AB   Racemic as well as optically pure 2-azetidinone-tethered nitrones, both
     cyclic and acyclic, were smoothly prepared from 4-oxoazetidine-2-
     carbaldehydes.  The regio- and diastereoselectivities of the intermol.
     1,3-dipolar cycloaddn. reactions of 2-azetidinone-tethered nitrones with
     substituted alkenes and alkynes were investigated. 2-Azetidinone-tethered
     nitrones on reacting with various dipolarophiles yielded isoxazolinyl-,
     isoxazolidinyl-, or fused polycyclic-β-lactams, exhibiting good
     regio- and facial stereoselectivity in the most of the cases.  In addition,
     some interesting transformations of these cycloadducts were performed,
     yielding aziridinyl β-lactams or functionalized β-alkoxycarbonyl
```

γ-lactams (derivs. of the aza analog of paraconic acid).

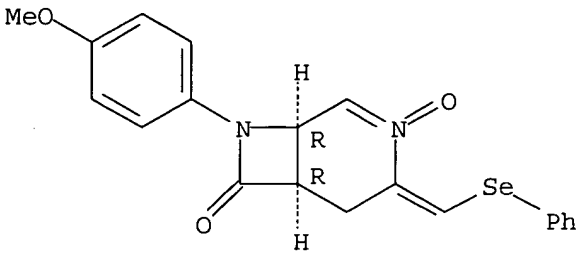
IT **474086-10-7P**

RL: SPN (Synthetic preparation); PREP (Preparation)
(stereoselective 1,3-dipolar cycloaddn. reactions of 2-azetidinone tethered nitrones with substituted alkenes and alkynes in preparation of highly functionalized β-lactams)

RN 474086-10-7 CAPLUS

CN 3,8-Diazabicyclo[4.2.0]oct-2-en-7-one, 8-(4-methoxyphenyl)-4-[(phenylseleno)methylene]-, 3-oxide, (1R,6R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry unknown.



RE.CNT 51 THERE ARE 51 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 2 OF 5 CAPLUS COPYRIGHT 2005 ACS on STN

AN 2001:798225 CAPLUS

DN 135:344471

TI Preparation of diazabicyclic compounds as central nervous system active agents

IN Schrimpf, Michael R.; Tietje, Karin R.; Toupence, Richard B.; Ji, Jianguo; Basha, Anwer; Bunnelle, William H.; Daanen, Jerome F.; Pace, Jennifer M.; Sippy, Kevin B.

PA Abbott Laboratories, USA

SO PCT Int. Appl., 190 pp.
CODEN: PIXXD2

DT Patent

LA English

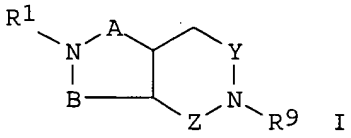
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2001081347	A2	20011101	WO 2001-US13798	20010427
	WO 2001081347	A3	20020131		
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
	RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
	US 2002019388	A1	20020214	US 2001-833914	20010412
	US 6809105	B2	20041026		
	CA 2407094	AA	20011101	CA 2001-2407094	20010427

	BR 2001007246	A	20021001	BR 2001-7246	20010427
	EP 1284976	A2	20030226	EP 2001-944118	20010427
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
	JP 2003531210	T2	20031021	JP 2001-578437	20010427
	NZ 521734	A	20041029	NZ 2001-521734	20010427
	ZA 2002008274	A	20040211	ZA 2002-8274	20021014
	NO 2002005107	A	20021219	NO 2002-5107	20021024
	BG 107303	A	20030731	BG 2002-107303	20021121
	US 2004186107	A1	20040923	US 2004-810999	20040326
PRAI	US 2000-200111P	P	20000427		
	US 2000-559943	A	20000427		
	US 2001-833914	A	20010412		
	WO 2001-US13798	W	20010427		

OS MARPAT 135:344471

GI



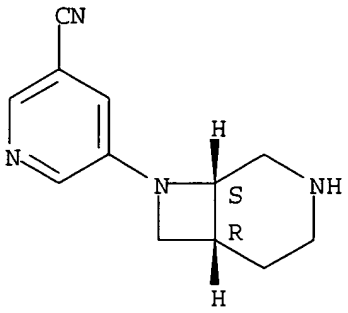
I

AB Diazabicyclic compds. (I; e.g. cis-2-(3-pyridinyl)octahydropyrrolo[3,4-c]pyrrole dihydrochloride), pharmaceutical compns. of these compds., and use of said compns. to control synaptic transmission in mammals are claimed. In I: A = covalent bond, CH2, CH2CH2, and CH2CH2CH2; B = CH2 and CH2CH2, provided that when A is CH2CH2CH2, then B is CH2; Y = covalent bond, CH2, and CH2CH2; Z = covalent bond, CH2, and CH2CH2, provided that when Y is CH2CH2, then Z is a covalent bond and further provided that when Z is CH2CH2, then Y is a covalent bond. R1 = optionally substituted phthalazin-1-yl, pyridin-3-yl, pyrazinyl, pyrimidin-5-yl, pyridazin-3-yl, quinolin-3-yl, thieno[3,2-b]pyridin-2-yl, furano[3,2-b]pyridin-2-yl, thieno[3,2-b]pyridin-3-yl, furano[3,2-b]pyridin-3-yl, furano[3,2-b]pyridin-6-yl, thieno[3,2-b]pyridin-6-yl, furano[2,3-b]pyridin-5-yl, thieno[2,3-b]pyridin-5-yl, isothiazol-5-yl, isoxazol-5-yl. R9 = H, alkoxycarbonyl, alkyl, amino, aminoalkyl, aminocarbonylalkyl, benzyloxycarbonyl, cyanoalkyl, dihydro-3-pyridinylcarbonyl, hydroxy, hydroxyalkyl, and phenoxycarbonyl. Values are reported for nicotinic acetylcholine receptor binding potencies and effectiveness of nicotinic acetylcholine receptor ligands as analgesic agents and in the formalin test for some of the claimed compds. Ninety-six example prepns. are given but the methods of preparation are not claimed. The crystal and mol. structures of (3aS,6aS)-5-[(4-nitrophenyl)sulfonyl]-1-((1R)-1-phenylethyl)octahydropyrrolo[3,4-b]pyrrole and tert-Bu (3S,4S)-4-(hydroxymethyl)-3-[((1S)-1-phenylethyl)amino]-1-piperidinecarboxylate were determined by x-ray crystallog.

IT **370881-88-2P**, 5-((1S,6R)-3,8-Diazabicyclo[4.2.0]oct-8-yl)nicotinonitrile
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(intermediate; preparation of diazabicyclic compds. as central nervous

system active agents)
RN 370881-88-2 CAPLUS
CN 3-Pyridinecarbonitrile, 5-(1S,6R)-3,8-diazabicyclo[4.2.0]oct-8-yl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

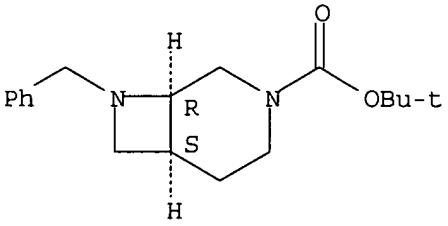


IT **370880-60-7P**, tert-Butyl cis-8-benzyl 3,8-diazabicyclo[4.2.0]octane-3-carboxylate **370880-62-9P**, cis-8-Benzyl-3,8-diazabicyclo[4.2.0]octane mono(4-methylbenzenesulfonate) **370880-63-0P**, cis-8-Benzyl-3-(3-pyridinyl)-3,8-diazabicyclo[4.2.0]octane **370880-97-0P**, tert-Butyl cis-8-[(2-nitrophenyl)sulfonyl]-3,8-diazabicyclo[4.2.0]octane-3-carboxylate **370880-98-1P**, Benzyl cis-8-[(2-nitrophenyl)sulfonyl]-3,8-diazabicyclo[4.2.0]octane-3-carboxylate **370880-99-2P**, Benzyl cis-8-(tert-butoxycarbonyl)-3,8-diazabicyclo[4.2.0]octane-3-carboxylate **370881-00-8P**, tert-Butyl cis-3,8-diazabicyclo[4.2.0]octane-8-carboxylate **370881-01-9P**, tert-Butyl cis-3-(6-chloro-3-pyridinyl)-3,8-diazabicyclo[4.2.0]octane-8-carboxylate **370881-06-4P**, tert-Butyl cis-3,8-diazabicyclo[4.2.0]octane-3-carboxylate **370881-07-5P**, tert-Butyl cis-8-(3-pyridinyl)-3,8-diazabicyclo[4.2.0]octane-3-carboxylate **370881-10-0P**, tert-Butyl cis-8-(6-chloro-3-pyridinyl)-3,8-diazabicyclo[4.2.0]octane-3-carboxylate **370881-16-6P**, tert-Butyl (1S,6R)-8-(6-chloro-3-pyridinyl)-3,8-diazabicyclo[4.2.0]octane-3-carboxylate **370881-19-9P**, tert-Butyl (1R,6S)-8-(6-chloro-3-pyridinyl)-3,8-diazabicyclo[4.2.0]octane-3-carboxylate **370881-22-4P**, tert-Butyl (1R,6S)-3,8-diazabicyclo[4.2.0]octane-8-carboxylate **370881-23-5P**, tert-Butyl (1R,6S)-3-(6-chloro-3-pyridinyl)-3,8-diazabicyclo[4.2.0]octane-8-carboxylate **370881-27-9P**, tert-Butyl (1R,6S)-8-(5-cyano-3-pyridinyl)-3,8-diazabicyclo[4.2.0]octane-3-carboxylate **370881-95-1P**, tert-Butyl (1S,6R)-8-[(2-nitrophenyl)sulfonyl]-3,8-diazabicyclo[4.2.0]octane-3-carboxylate **370881-96-2P**, tert-Butyl (1S,6R)-3,8-diazabicyclo[4.2.0]octane-3-carboxylate **370881-97-3P**, tert-Butyl (1S,6R)-8-(5-cyano-3-pyridinyl)-3,8-diazabicyclo[4.2.0]octane-3-carboxylate **370882-01-2P**, tert-Butyl cis-3-(5-cyano-3-pyridinyl)-3,8-diazabicyclo[4.2.0]octane-8-carboxylate **370882-90-9P**, (1S,6R)-8-(5-Methoxy-3-pyridinyl)-3,8-diazabicyclo[4.2.0]octane **370882-92-1P**, tert-Butyl (1S,6R)-8-(5-methoxy-3-pyridinyl)-3,8-diazabicyclo[4.2.0]octane-3-carboxylate **370882-93-2P**, (1S,6R)-8-(6-Chloro-5-methyl-3-pyridinyl)-3,8-diazabicyclo[4.2.0]octane **370882-95-4P**, tert-Butyl (1S,6R)-8-(6-chloro-5-methyl-3-pyridinyl)-3,8-diazabicyclo[4.2.0]octane-3-carboxylate **370882-96-5P**,

(1R,6S)-8-(6-Chloro-5-methyl-3-pyridinyl)-3,8-diazabicyclo[4.2.0]octane **370882-98-7P**, tert-Butyl (1R,6S)-8-[(2-nitrophenyl)sulfonyl]-3,8-diazabicyclo[4.2.0]octane-3-carboxylate **370882-99-8P**, tert-Butyl (1R,6S)-3,8-diazabicyclo[4.2.0]octane-3-carboxylate **370883-00-4P**, tert-Butyl (1R,6S)-8-(6-chloro-5-methyl-3-pyridinyl)-3,8-diazabicyclo[4.2.0]octane-3-carboxylate **370883-01-5P**, (1S,6R)-8-(3-Pyridinyl)-3,8-diazabicyclo[4.2.0]octane **370883-03-7P**, tert-Butyl (1S,6R)-8-(3-pyridinyl)-3,8-diazabicyclo[4.2.0]octane-3-carboxylate **370883-04-8P**, (1R,6S)-8-(3-Pyridinyl)-3,8-diazabicyclo[4.2.0]octane **370883-06-0P**, tert-Butyl (1R,6S)-8-(3-pyridinyl)-3,8-diazabicyclo[4.2.0]octane-3-carboxylate **370883-07-1P**, (1S,6R)-8-(5,6-Dichloro-3-pyridinyl)-3,8-diazabicyclo[4.2.0]octane **370883-09-3P**, tert-Butyl (1S,6R)-8-(5,6-dichloro-3-pyridinyl)-3,8-diazabicyclo[4.2.0]octane-3-carboxylate **370883-10-6P**, (1R,6S)-8-(5,6-Dichloro-3-pyridinyl)-3,8-diazabicyclo[4.2.0]octane **370883-12-8P**, tert-Butyl (1R,6S)-8-(5,6-dichloro-3-pyridinyl)-3,8-diazabicyclo[4.2.0]octane-3-carboxylate
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(intermediate; preparation of diazabicyclic compds. as central nervous system active agents)

RN 370880-60-7 CAPLUS
CN 3,8-Diazabicyclo[4.2.0]octane-3-carboxylic acid, 8-(phenylmethyl)-, 1,1-dimethylethyl ester, (1R,6S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

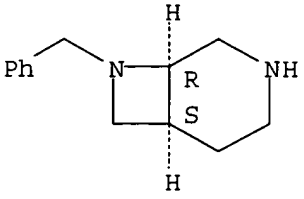


RN 370880-62-9 CAPLUS
CN 3,8-Diazabicyclo[4.2.0]octane, 8-(phenylmethyl)-, (1R,6S)-rel-, 4-methylbenzenesulfonate (9CI) (CA INDEX NAME)

CM 1

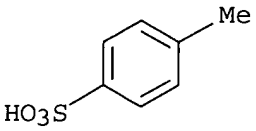
CRN 370880-61-8
CMF C13 H18 N2

Relative stereochemistry.



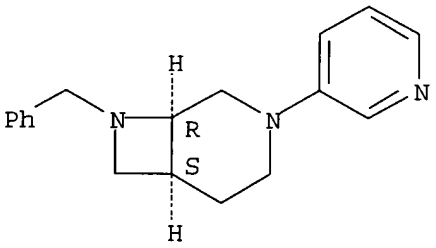
CM 2

CRN 104-15-4
CMF C7 H8 O3 S



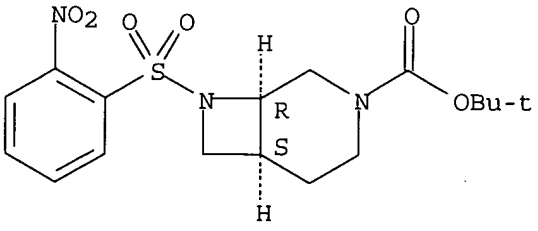
RN 370880-63-0 CAPLUS
CN 3,8-Diazabicyclo[4.2.0]octane, 8-(phenylmethyl)-3-(3-pyridinyl)-, (1R,6S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



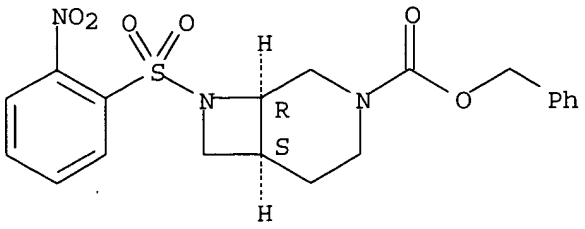
RN 370880-97-0 CAPLUS
CN 3,8-Diazabicyclo[4.2.0]octane-3-carboxylic acid, 8-[(2-nitrophenyl)sulfonyl]-, 1,1-dimethylethyl ester, (1R,6S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



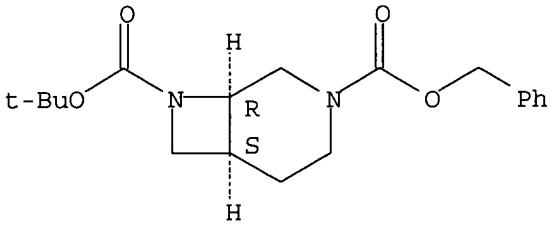
RN 370880-98-1 CAPLUS
CN 3,8-Diazabicyclo[4.2.0]octane-3-carboxylic acid, 8-[(2-nitrophenyl)sulfonyl]-, phenylmethyl ester, (1R,6S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



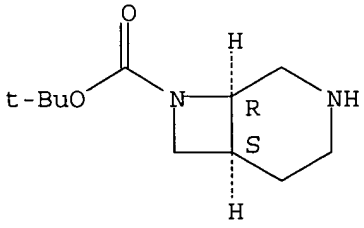
RN 370880-99-2 CAPLUS
CN 3,8-Diazabicyclo[4.2.0]octane-3,8-dicarboxylic acid, 8-(1,1-dimethylethyl) 3-(phenylmethyl) ester, (1R,6S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



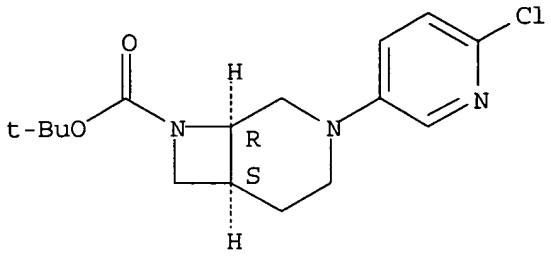
RN 370881-00-8 CAPLUS
CN 3,8-Diazabicyclo[4.2.0]octane-8-carboxylic acid, 1,1-dimethylethyl ester, (1R,6S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



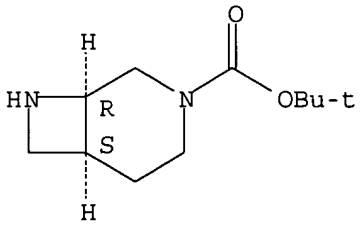
RN 370881-01-9 CAPLUS
CN 3,8-Diazabicyclo[4.2.0]octane-8-carboxylic acid, 3-(6-chloro-3-pyridinyl)-, 1,1-dimethylethyl ester, (1R,6S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



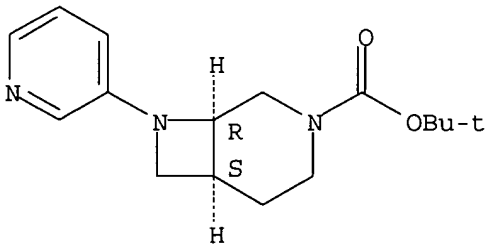
RN 370881-06-4 CAPLUS
CN 3,8-Diazabicyclo[4.2.0]octane-3-carboxylic acid, 1,1-dimethylethyl ester, (1R,6S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



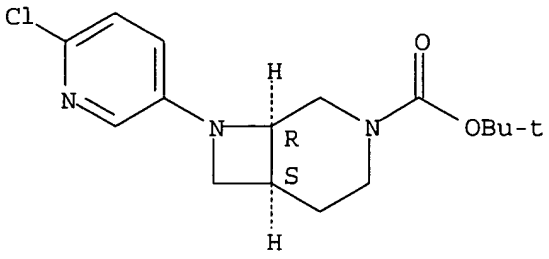
RN 370881-07-5 CAPLUS
CN 3,8-Diazabicyclo[4.2.0]octane-3-carboxylic acid, 8-(3-pyridinyl)-, 1,1-dimethylethyl ester, (1R,6S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



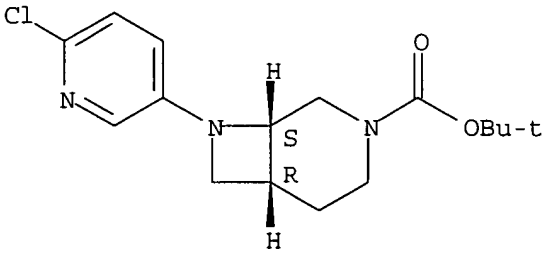
RN 370881-10-0 CAPLUS
CN 3,8-Diazabicyclo[4.2.0]octane-3-carboxylic acid, 8-(6-chloro-3-pyridinyl)-, 1,1-dimethylethyl ester, (1R,6S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



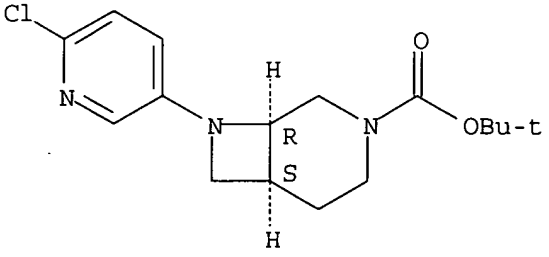
RN 370881-16-6 CAPLUS
CN 3,8-Diazabicyclo[4.2.0]octane-3-carboxylic acid, 8-(6-chloro-3-pyridinyl)-, 1,1-dimethylethyl ester, (1S,6R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



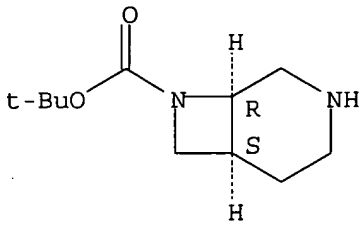
RN 370881-19-9 CAPLUS
CN 3,8-Diazabicyclo[4.2.0]octane-3-carboxylic acid, 8-(6-chloro-3-pyridinyl)-, 1,1-dimethylethyl ester, (1R,6S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



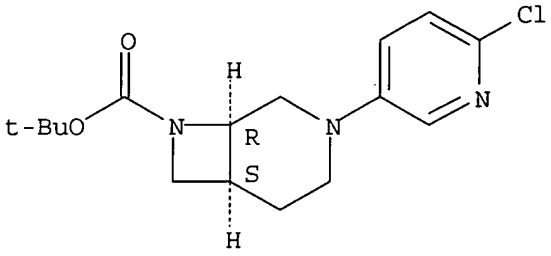
RN 370881-22-4 CAPLUS
CN 3,8-Diazabicyclo[4.2.0]octane-8-carboxylic acid, 1,1-dimethylethyl ester, (1R,6S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



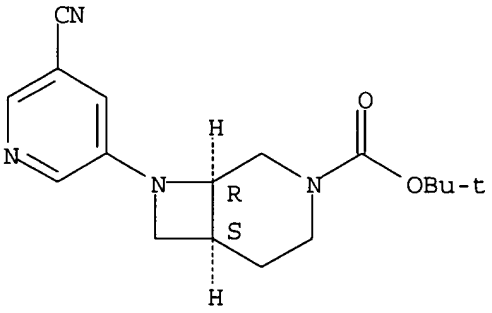
RN 370881-23-5 CAPLUS
CN 3,8-Diazabicyclo[4.2.0]octane-8-carboxylic acid, 3-(6-chloro-3-pyridinyl)-, 1,1-dimethylethyl ester, (1R,6S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



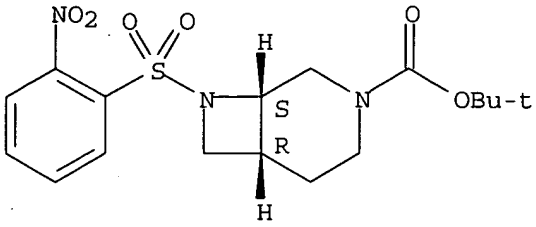
RN 370881-27-9 CAPLUS
CN 3,8-Diazabicyclo[4.2.0]octane-3-carboxylic acid, 8-(5-cyano-3-pyridinyl)-, 1,1-dimethylethyl ester, (1R,6S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



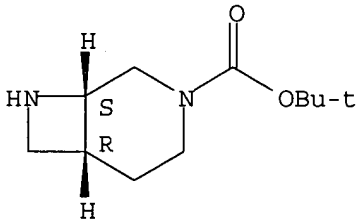
RN 370881-95-1 CAPLUS
CN 3,8-Diazabicyclo[4.2.0]octane-3-carboxylic acid, 8-[(2-nitrophenyl)sulfonyl]-, 1,1-dimethylethyl ester, (1S,6R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



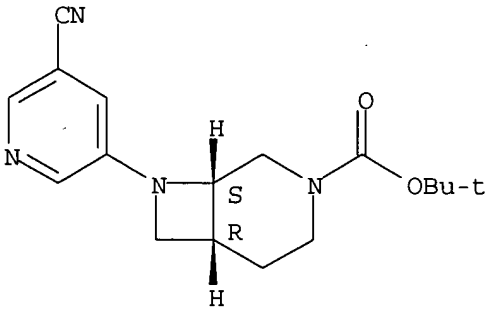
RN 370881-96-2 CAPLUS
CN 3,8-Diazabicyclo[4.2.0]octane-3-carboxylic acid, 1,1-dimethylethyl ester, (1S,6R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



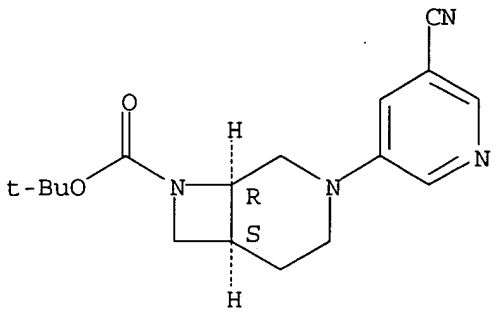
RN 370881-97-3 CAPLUS
CN 3,8-Diazabicyclo[4.2.0]octane-3-carboxylic acid, 8-(5-cyano-3-pyridinyl)-, 1,1-dimethylethyl ester, (1S,6R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



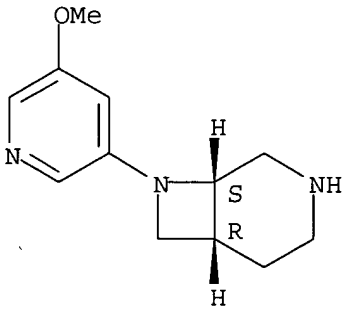
RN 370882-01-2 CAPLUS
CN 3,8-Diazabicyclo[4.2.0]octane-8-carboxylic acid, 3-(5-cyano-3-pyridinyl)-, 1,1-dimethylethyl ester, (1R,6S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



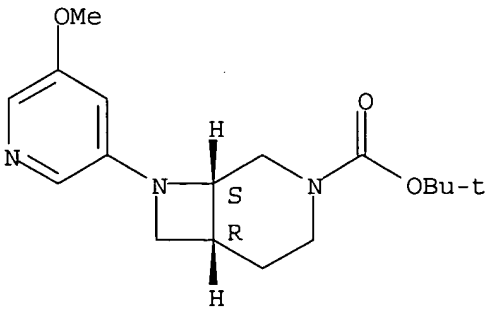
RN 370882-90-9 CAPLUS
CN 3,8-Diazabicyclo[4.2.0]octane, 8-(5-methoxy-3-pyridinyl)-, (1S,6R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



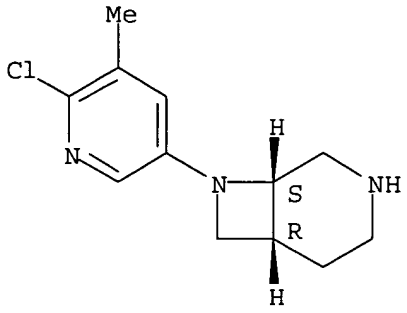
RN 370882-92-1 CAPLUS
CN 3,8-Diazabicyclo[4.2.0]octane-3-carboxylic acid, 8-(5-methoxy-3-pyridinyl)-, 1,1-dimethylethyl ester, (1S,6R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



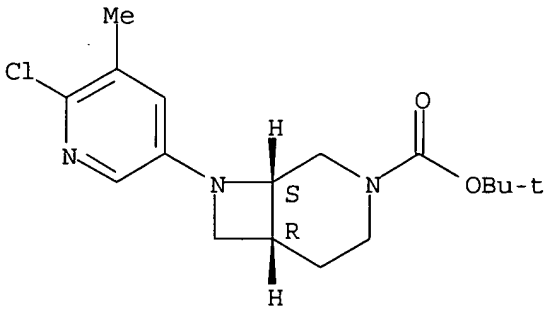
RN 370882-93-2 CAPLUS
CN 3,8-Diazabicyclo[4.2.0]octane, 8-(6-chloro-5-methyl-3-pyridinyl)-, (1S,6R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



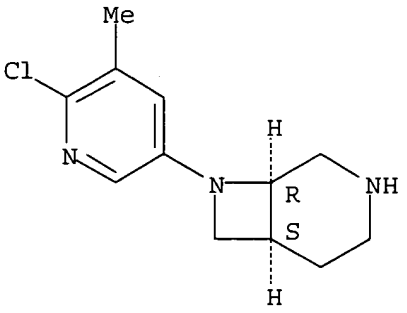
RN 370882-95-4 CAPLUS
CN 3,8-Diazabicyclo[4.2.0]octane-3-carboxylic acid, 8-(6-chloro-5-methyl-3-pyridinyl)-, 1,1-dimethylethyl ester, (1S,6R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 370882-96-5 CAPLUS
CN 3,8-Diazabicyclo[4.2.0]octane, 8-(6-chloro-5-methyl-3-pyridinyl)-, (1R,6S)- (9CI) (CA INDEX NAME)

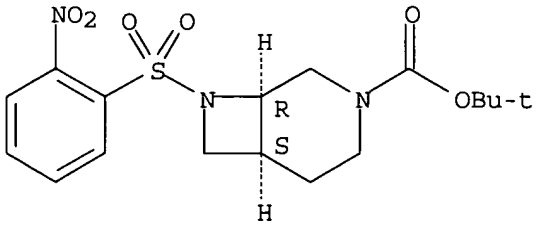
Absolute stereochemistry.



RN 370882-98-7 CAPLUS
CN 3,8-Diazabicyclo[4.2.0]octane-3-carboxylic acid, 8-[(2-

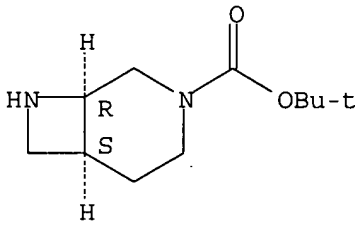
nitrophenyl)sulfonyl]-, 1,1-dimethylethyl ester, (1R,6S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



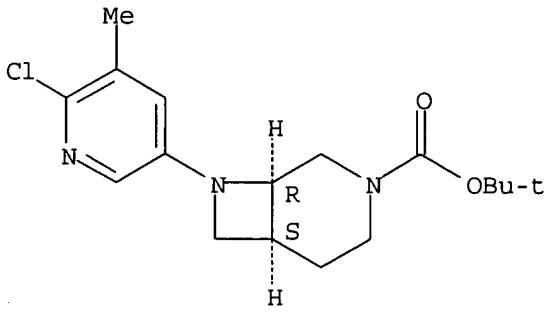
RN 370882-99-8 CAPLUS
CN 3,8-Diazabicyclo[4.2.0]octane-3-carboxylic acid, 1,1-dimethylethyl ester, (1R,6S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



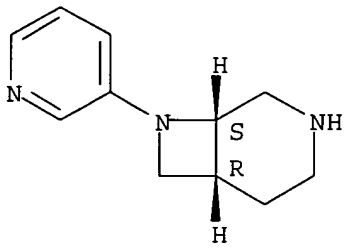
RN 370883-00-4 CAPLUS
CN 3,8-Diazabicyclo[4.2.0]octane-3-carboxylic acid, 8-(6-chloro-5-methyl-3-pyridinyl)-, 1,1-dimethylethyl ester, (1R,6S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



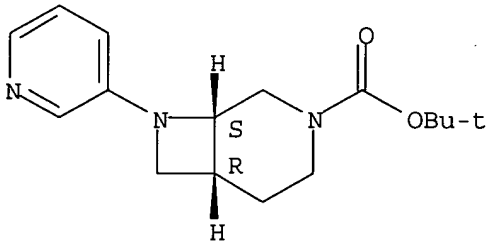
RN 370883-01-5 CAPLUS
CN 3,8-Diazabicyclo[4.2.0]octane, 8-(3-pyridinyl)-, (1S,6R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



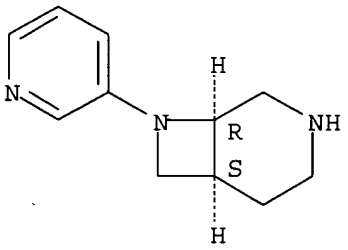
RN 370883-03-7 CAPLUS
CN 3,8-Diazabicyclo[4.2.0]octane-3-carboxylic acid, 8-(3-pyridinyl)-, 1,1-dimethylethyl ester, (1S,6R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



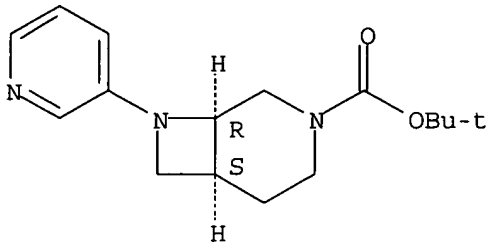
RN 370883-04-8 CAPLUS
CN 3,8-Diazabicyclo[4.2.0]octane, 8-(3-pyridinyl)-, (1R,6S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



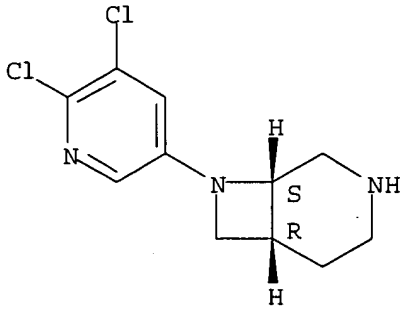
RN 370883-06-0 CAPLUS
CN 3,8-Diazabicyclo[4.2.0]octane-3-carboxylic acid, 8-(3-pyridinyl)-, 1,1-dimethylethyl ester, (1R,6S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



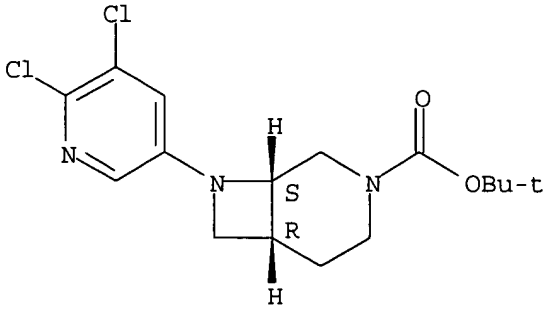
RN 370883-07-1 CAPLUS
CN 3,8-Diazabicyclo[4.2.0]octane, 8-(5,6-dichloro-3-pyridinyl)-, (1S,6R)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.



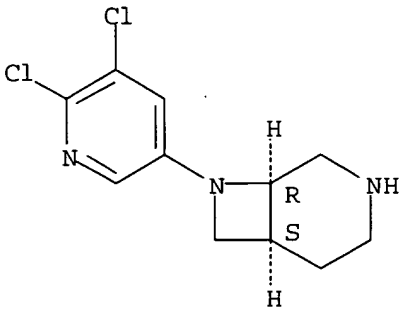
RN 370883-09-3 CAPLUS
CN 3,8-Diazabicyclo[4.2.0]octane-3-carboxylic acid, 8-(5,6-dichloro-3-pyridinyl)-, 1,1-dimethylethyl ester, (1S,6R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



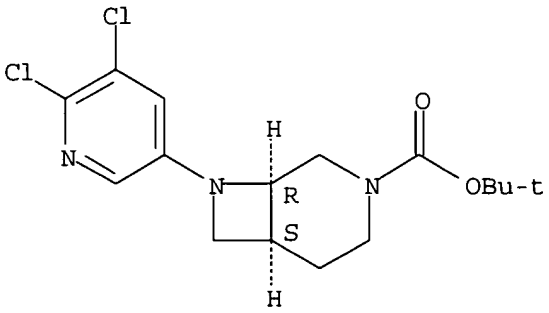
RN 370883-10-6 CAPLUS
CN 3,8-Diazabicyclo[4.2.0]octane, 8-(5,6-dichloro-3-pyridinyl)-, (1R,6S)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 370883-12-8 CAPLUS
CN 3,8-Diazabicyclo[4.2.0]octane-3-carboxylic acid, 8-(5,6-dichloro-3-pyridinyl)-, 1,1-dimethylethyl ester, (1R,6S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

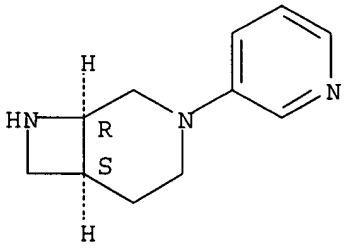


IT **370880-57-2P**, cis-3-(3-Pyridinyl)-3,8-diazabicyclo[4.2.0]octane **370880-58-3P**, cis-3-(3-Pyridinyl)-3,8-diazabicyclo[4.2.0]octane tris(4-methylbenzenesulfonate) **370880-93-6P**, cis-3-(6-Chloro-3-pyridinyl)-3,8-diazabicyclo[4.2.0]octane **370880-94-7P**, cis-3-(6-Chloro-3-pyridinyl)-3,8-diazabicyclo[4.2.0]octane bis(4-methylbenzenesulfonate) **370881-04-2P**, cis-8-(3-Pyridinyl)-3,8-diazabicyclo[4.2.0]octane **370881-05-3P**, cis-8-(3-Pyridinyl)-3,8-diazabicyclo[4.2.0]octane bis(4-methylbenzenesulfonate) **370881-08-6P**, cis-8-(6-Chloro-3-pyridinyl)-3,8-diazabicyclo[4.2.0]octane **370881-09-7P**, cis-8-(6-Chloro-3-pyridinyl)-3,8-diazabicyclo[4.2.0]octane bis(4-methylbenzenesulfonate) **370881-14-4P**, (1S,6R)-cis-8-(6-Chloro-3-pyridinyl)-3,8-diazabicyclo[4.2.0]octane **370881-15-5P**, (1S,6R)-8-(6-Chloro-3-pyridinyl)-3,8-diazabicyclo[4.2.0]octane difumarate **370881-18-8P**, (1R,6S)-8-(6-Chloro-3-pyridinyl)-3,8-diazabicyclo[4.2.0]octane difumarate **370881-20-2P**, (1R,6S)-3-(6-Chloro-3-pyridinyl)-3,8-diazabicyclo[4.2.0]octane **370881-21-3P**, (1R,6S)-3-(6-Chloro-3-pyridinyl)-3,8-diazabicyclo[4.2.0]octane fumarate (10:11) **370881-24-6P**, 5-[(1R,6S)-3,8-Diazabicyclo[4.2.0]oct-8-yl]nicotinonitrile **370881-25-7P**, 5-[(1R,6S)-3,8-Diazabicyclo[4.2.0]oct-8-yl]nicotinonitrile fumarate (10:3) **370881-89-3P**, 5-[(1S,6R)-3,8-Diazabicyclo[4.2.0]oct-8-yl]nicotinonitrile monofumarate **370881-98-4P**, cis-5-(3,8-Diazabicyclo[4.2.0]oct-3-

yl)nicotinonitrile **370881-99-5P**, cis-5-(3,8-Diazabicyclo[4.2.0]oct-3-yl)nicotinonitrile fumarate (2:3) **370882-91-0P**, (1S,6R)-8-(5-Methoxy-3-pyridinyl)-3,8-diazabicyclo[4.2.0]octane monofumarate **370882-94-3P**, (1S,6R)-8-(6-Chloro-5-methyl-3-pyridinyl)-3,8-diazabicyclo[4.2.0]octane fumarate (10:13) **370882-97-6P**, (1R,6S)-8-(6-Chloro-5-methyl-3-pyridinyl)-3,8-diazabicyclo[4.2.0]octane fumarate (5:8) **370883-02-6P**, (1S,6R)-8-(3-Pyridinyl)-3,8-diazabicyclo[4.2.0]octane mono(4-methylbenzenesulfonate) **370883-05-9P**, (1R,6S)-8-(3-Pyridinyl)-3,8-diazabicyclo[4.2.0]octane mono(4-methylbenzenesulfonate) **370883-08-2P**, (1S,6R)-8-(5,6-Dichloro-3-pyridinyl)-3,8-diazabicyclo[4.2.0]octane mono(4-methylbenzenesulfonate) **370883-11-7P**, (1R,6S)-8-(5,6-Dichloro-3-pyridinyl)-3,8-diazabicyclo[4.2.0]octane mono(4-methylbenzenesulfonate) **370883-31-1P**, cis-8-(5-Methoxy-3-pyridinyl)-3,8-diazabicyclo[4.2.0]octane **370883-32-2P**, (1R,6S)-8-(5-Methoxy-3-pyridinyl)-3,8-diazabicyclo[4.2.0]octane **370883-33-3P**, cis-8-(6-Chloro-5-methyl-3-pyridinyl)-3,8-diazabicyclo[4.2.0]octane **370883-34-4P**, cis-8-(5,6-Dichloro-3-pyridinyl)-3,8-diazabicyclo[4.2.0]octane
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of diazabicyclic compds. as central nervous system active agents)

RN 370880-57-2 CAPLUS
CN 3,8-Diazabicyclo[4.2.0]octane, 3-(3-pyridinyl)-, (1R,6S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

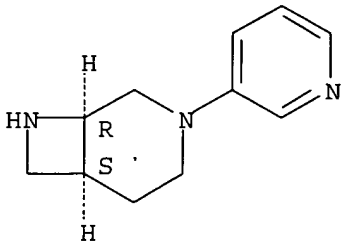


RN 370880-58-3 CAPLUS
CN 3,8-Diazabicyclo[4.2.0]octane, 3-(3-pyridinyl)-, (1R,6S)-rel-, tris(4-methylbenzenesulfonate) (9CI) (CA INDEX NAME)

CM 1

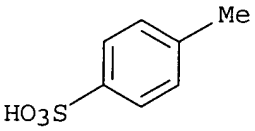
CRN 370880-57-2
CMF C11 H15 N3

Relative stereochemistry.



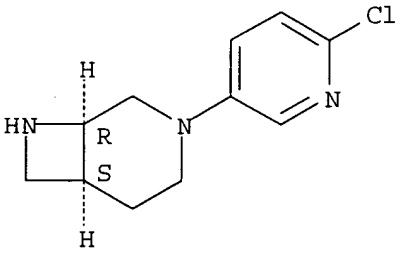
CM 2

CRN 104-15-4
CMF C7 H8 O3 S



RN 370880-93-6 CAPLUS
CN 3,8-Diazabicyclo[4.2.0]octane, 3-(6-chloro-3-pyridinyl)-, (1R,6S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

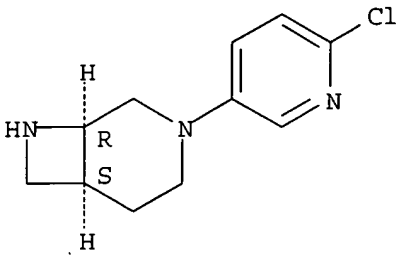


RN 370880-94-7 CAPLUS
CN 3,8-Diazabicyclo[4.2.0]octane, 3-(6-chloro-3-pyridinyl)-, (1R,6S)-rel-, bis(4-methylbenzenesulfonate) (9CI) (CA INDEX NAME)

CM 1

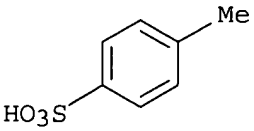
CRN 370880-93-6
CMF C11 H14 Cl N3

Relative stereochemistry.



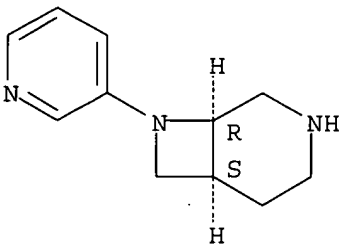
CM 2

CRN 104-15-4
CMF C7 H8 O3 S



RN 370881-04-2 CAPLUS
CN 3,8-Diazabicyclo[4.2.0]octane, 8-(3-pyridinyl)-, (1R,6S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

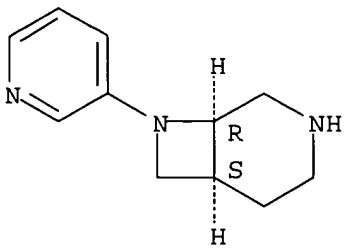


RN 370881-05-3 CAPLUS
CN 3,8-Diazabicyclo[4.2.0]octane, 8-(3-pyridinyl)-, (1R,6S)-rel-, bis(4-methylbenzenesulfonate) (9CI) (CA INDEX NAME)

CM 1

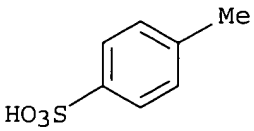
CRN 370881-04-2
CMF C11 H15 N3

Relative stereochemistry.



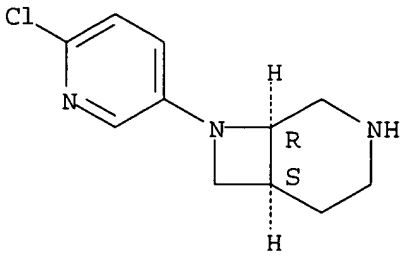
CM 2

CRN 104-15-4
CMF C7 H8 O3 S



RN 370881-08-6 CAPLUS
CN 3,8-Diazabicyclo[4.2.0]octane, 8-(6-chloro-3-pyridinyl)-, (1R,6S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

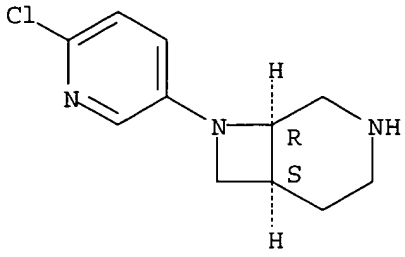


RN 370881-09-7 CAPLUS
CN 3,8-Diazabicyclo[4.2.0]octane, 8-(6-chloro-3-pyridinyl)-, (1R,6S)-rel-, bis(4-methylbenzenesulfonate) (9CI) (CA INDEX NAME)

CM 1

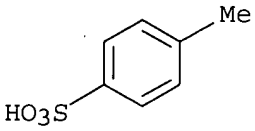
CRN 370881-08-6
CMF C11 H14 Cl N3

Relative stereochemistry.



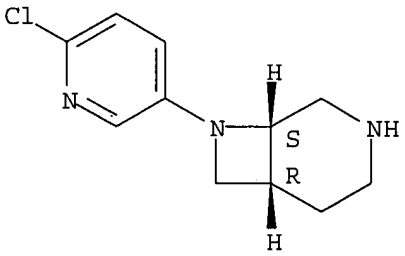
CM 2

CRN 104-15-4
CMF C7 H8 O3 S



RN 370881-14-4 CAPLUS
CN 3,8-Diazabicyclo[4.2.0]octane, 8-(6-chloro-3-pyridinyl)-, (1S,6R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

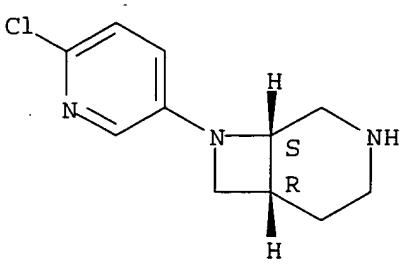


RN 370881-15-5 CAPLUS
CN 3,8-Diazabicyclo[4.2.0]octane, 8-(6-chloro-3-pyridinyl)-, (1S,6R)-, (2E)-2-butenedioate (1:2) (9CI) (CA INDEX NAME)

CM 1

CRN 370881-14-4
CMF C11 H14 Cl N3

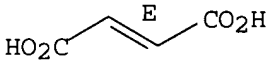
Absolute stereochemistry.



CM 2

CRN 110-17-8
CMF C4 H4 O4

Double bond geometry as shown.

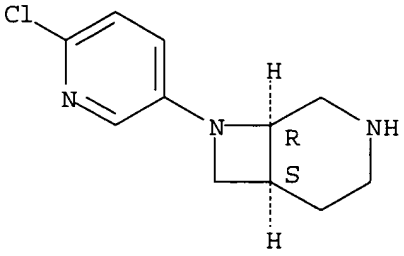


RN 370881-18-8 CAPLUS
CN 3,8-Diazabicyclo[4.2.0]octane, 8-(6-chloro-3-pyridinyl)-, (1R,6S)-, (2E)-2-butenedioate (1:2) (9CI) (CA INDEX NAME)

CM 1

CRN 370881-17-7
CMF C11 H14 Cl N3

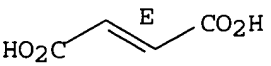
Absolute stereochemistry.



CM 2

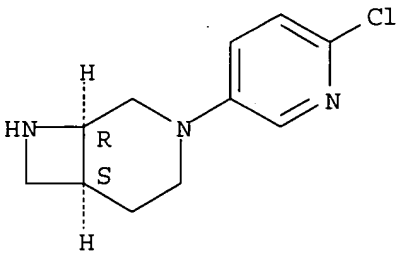
CRN 110-17-8
CMF C4 H4 O4

Double bond geometry as shown.



RN 370881-20-2 CAPLUS
CN 3,8-Diazabicyclo[4.2.0]octane, 3-(6-chloro-3-pyridinyl)-, (1R,6S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

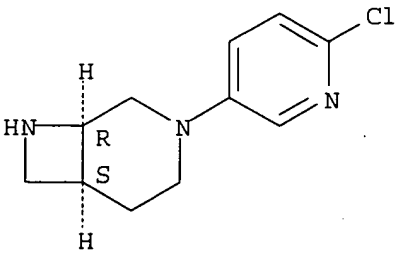


RN 370881-21-3 CAPLUS
CN 3,8-Diazabicyclo[4.2.0]octane, 3-(6-chloro-3-pyridinyl)-, (1R,6S)-, (2E)-2-butenedioate (10:11) (9CI) (CA INDEX NAME)

CM 1

CRN 370881-20-2
CMF C11 H14 Cl N3

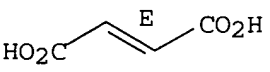
Absolute stereochemistry.



CM 2

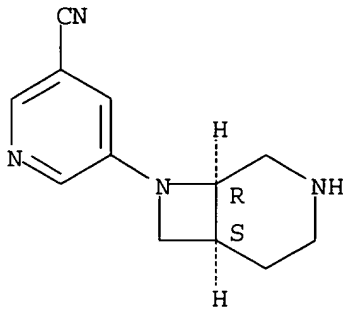
CRN 110-17-8
CMF C4 H4 O4

Double bond geometry as shown.



RN 370881-24-6 CAPLUS
CN 3-Pyridinecarbonitrile, 5-(1R,6S)-3,8-diazabicyclo[4.2.0]oct-8-yl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

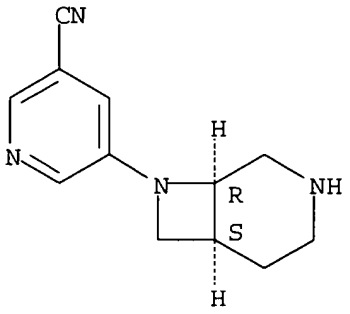


RN 370881-25-7 CAPLUS
CN 3-Pyridinecarbonitrile, 5-(1R,6S)-3,8-diazabicyclo[4.2.0]oct-8-yl-, (2E)-2-butenedioate (10:3) (9CI) (CA INDEX NAME)

CM 1

CRN 370881-24-6
CMF C12 H14 N4

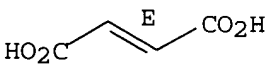
Absolute stereochemistry.



CM 2

CRN 110-17-8
CMF C4 H4 O4

Double bond geometry as shown.

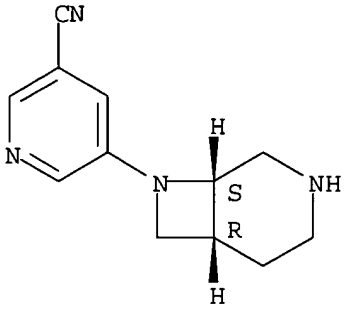


RN 370881-89-3 CAPLUS
CN 3-Pyridinecarbonitrile, 5-(1S,6R)-3,8-diazabicyclo[4.2.0]oct-8-yl-, (2E)-2-butenedioate (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 370881-88-2
CMF C12 H14 N4

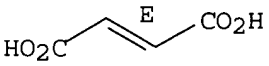
Absolute stereochemistry.



CM 2

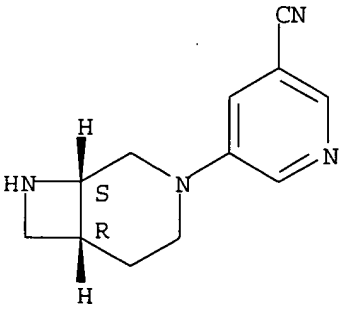
CRN 110-17-8
CMF C4 H4 O4

Double bond geometry as shown.



RN 370881-98-4 CAPLUS
CN 3-Pyridinecarbonitrile, 5-(1R,6S)-3,8-diazabicyclo[4.2.0]oct-3-yl-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

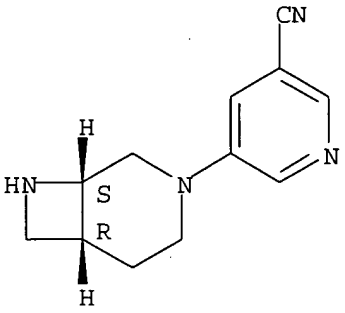


RN 370881-99-5 CAPLUS
CN 3-Pyridinecarbonitrile, 5-[(1R,6S)-3,8-diazabicyclo[4.2.0]oct-3-yl]-, rel-, (2E)-2-butenedioate (2:3) (9CI) (CA INDEX NAME)

CM 1

CRN 370881-98-4
CMF C12 H14 N4

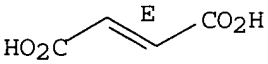
Relative stereochemistry.



CM 2

CRN 110-17-8
CMF C4 H4 O4

Double bond geometry as shown.

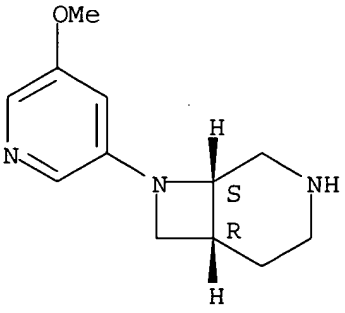


RN 370882-91-0 CAPLUS
CN 3,8-Diazabicyclo[4.2.0]octane, 8-(5-methoxy-3-pyridinyl)-, (1S,6R)-, (2E)-2-butenedioate (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 370882-90-9
CMF C12 H17 N3 O

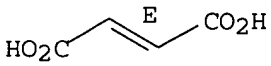
Absolute stereochemistry.



CM 2

CRN 110-17-8
CMF C4 H4 O4

Double bond geometry as shown.

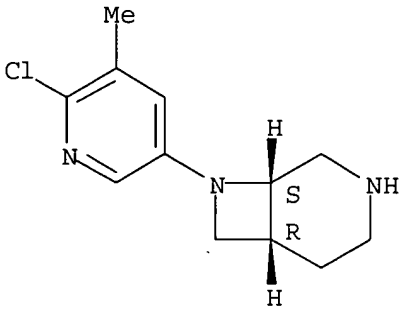


RN 370882-94-3 CAPLUS
CN 3,8-Diazabicyclo[4.2.0]octane, 8-(6-chloro-5-methyl-3-pyridinyl)-, (1S,6R)-, (2E)-2-butenedioate (10:13) (9CI) (CA INDEX NAME)

CM 1

CRN 370882-93-2
CMF C12 H16 Cl N3

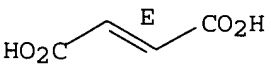
Absolute stereochemistry.



CM 2

CRN 110-17-8
CMF C4 H4 O4

Double bond geometry as shown.

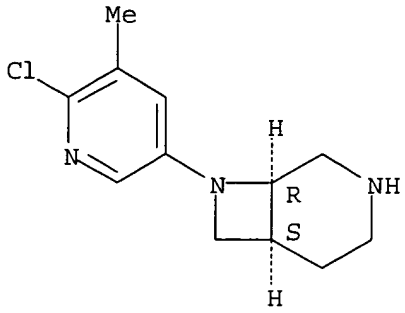


RN 370882-97-6 CAPLUS
CN 3,8-Diazabicyclo[4.2.0]octane, 8-(6-chloro-5-methyl-3-pyridinyl)-, (1R,6S)-, (2E)-2-butenedioate (5:8) (9CI) (CA INDEX NAME)

CM 1

CRN 370882-96-5
CMF C12 H16 Cl N3

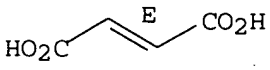
Absolute stereochemistry.



CM 2

CRN 110-17-8
CMF C4 H4 O4

Double bond geometry as shown.

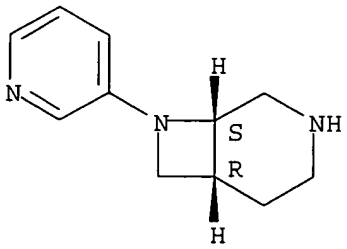


RN 370883-02-6 CAPLUS
CN 3,8-Diazabicyclo[4.2.0]octane, 8-(3-pyridinyl)-, (1S,6R)-, mono(4-methylbenzenesulfonate) (9CI) (CA INDEX NAME)

CM 1

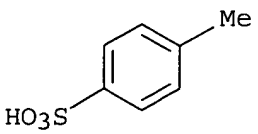
CRN 370883-01-5
CMF C11 H15 N3

Absolute stereochemistry.



CM 2

CRN 104-15-4
CMF C7 H8 O3 S

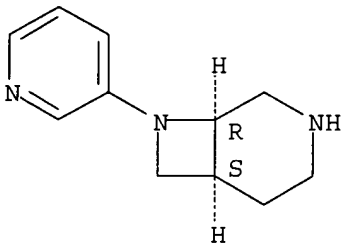


RN 370883-05-9 CAPLUS
CN 3,8-Diazabicyclo[4.2.0]octane, 8-(3-pyridinyl)-, (1R,6S)-, mono(4-methylbenzenesulfonate) (9CI) (CA INDEX NAME)

CM 1

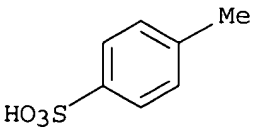
CRN 370883-04-8
CMF C11 H15 N3

Absolute stereochemistry.



CM 2

CRN 104-15-4
CMF C7 H8 O3 S

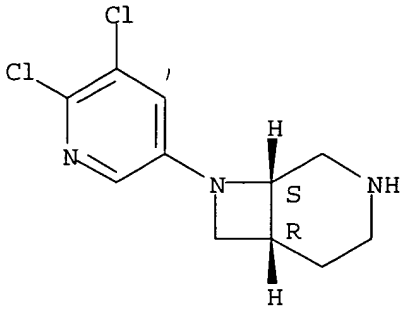


RN 370883-08-2 CAPLUS
CN 3,8-Diazabicyclo[4.2.0]octane, 8-(5,6-dichloro-3-pyridinyl)-, (1S,6R)-, mono(4-methylbenzenesulfonate) (9CI) (CA INDEX NAME)

CM 1

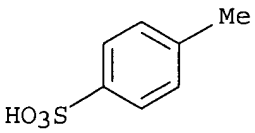
CRN 370883-07-1
CMF C11 H13 Cl2 N3

Absolute stereochemistry.



CM 2

CRN 104-15-4
CMF C7 H8 O3 S

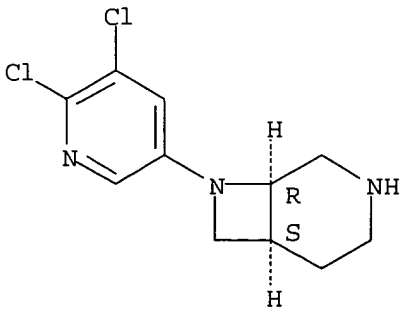


RN 370883-11-7 CAPLUS
CN 3,8-Diazabicyclo[4.2.0]octane, 8-(5,6-dichloro-3-pyridinyl)-, (1R,6S)-, mono(4-methylbenzenesulfonate) (9CI) (CA INDEX NAME)

CM 1

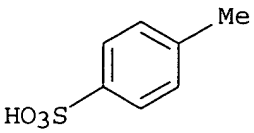
CRN 370883-10-6
CMF C11 H13 Cl2 N3

Absolute stereochemistry.



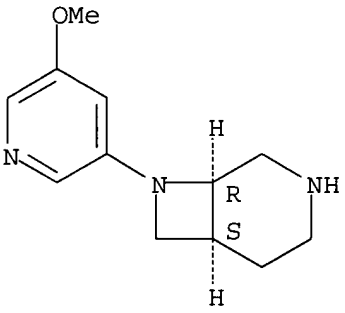
CM 2

CRN 104-15-4
CMF C7 H8 O3 S



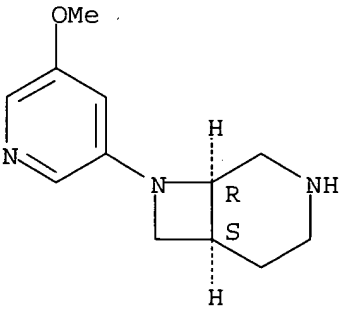
RN 370883-31-1 CAPLUS
CN 3,8-Diazabicyclo[4.2.0]octane, 8-(5-methoxy-3-pyridinyl)-, (1R,6S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



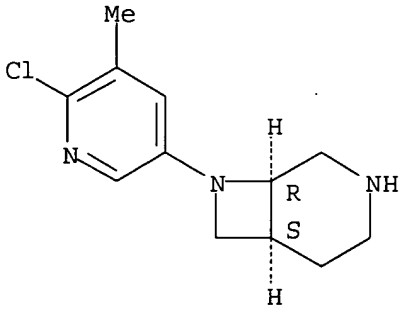
RN 370883-32-2 CAPLUS
CN 3,8-Diazabicyclo[4.2.0]octane, 8-(5-methoxy-3-pyridinyl)-, (1R,6S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



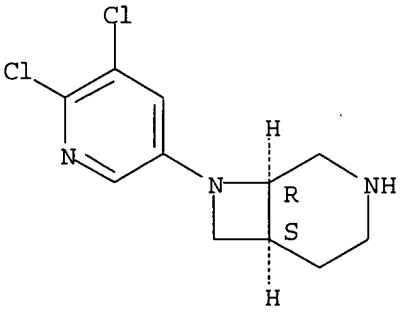
RN 370883-33-3 CAPLUS
CN 3,8-Diazabicyclo[4.2.0]octane, 8-(6-chloro-5-methyl-3-pyridinyl)-, (1R,6S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 370883-34-4 CAPLUS
CN 3,8-Diazabicyclo[4.2.0]octane, 8-(5,6-dichloro-3-pyridinyl)-, (1R,6S)-rel-(9CI) (CA INDEX NAME)

Relative stereochemistry.



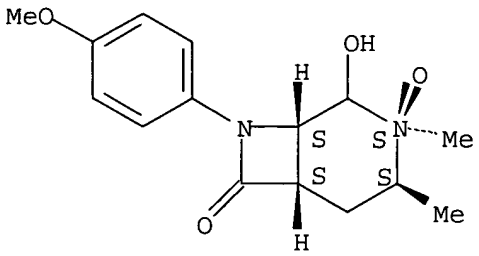
L11 ANSWER 3 OF 5 CAPLUS COPYRIGHT 2005 ACS on STN
AN 1999:448468 CAPLUS
DN 131:286290
TI Rapid entry to enantiopure polycyclic β-lactams via intramolecular nitrone-alkene cycloaddition of 2-azetidinone-tethered alkenylaldehydes
AU Alcaide, Benito; Alonso, Jose M.; Aly, Moustafa F.; Saez, Elena; Martinez-Alcazar, M. Paz; Hernandez-Cano, Felix
CS Departamento de Quimica Organica I, Facultad de Quimica, Universidad Complutense, Madrid, 28040, Spain
SO Tetrahedron Letters (1999), 40(29), 5391-5394
CODEN: TELEAY; ISSN: 0040-4039
PB Elsevier Science Ltd.
DT Journal
LA English
OS CASREACT 131:286290
AB New enantiomerically pure fused or bridged polycyclic β-lactam systems are regio- and stereoselectively prepared via intramol. nitrone-alkene cycloaddn. of 2-azetidinone-tethered alkenyl aldehydes. The regioselectivity of the cycloaddn. can be tuned by moving the alkene substituent from N-1 to C-3 on the 2-azetidinone ring.
IT **246031-59-4P**

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of polycyclic β-lactams via intramol. nitrone-alkene cycloaddn. of alkenylazetidinecarboxaldehydes)

RN 246031-59-4 CAPLUS

CN 3,8-Diazabicyclo[4.2.0]octan-7-one, 2-hydroxy-8-(4-methoxyphenyl)-3,4-dimethyl-, 3-oxide, (1R,3R,4R,6R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RE.CNT 37 THERE ARE 37 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 4 OF 5 CAPLUS COPYRIGHT 2005 ACS on STN

AN 1983:470489 CAPLUS

DN 99:70489

TI Thietones, oxetones and azetones

AU Wentrup, Curt; Gross, Gerhard

CS Fachbereich Chem., Univ. Marburg, Marburg, D-3550, Fed. Rep. Ger.

SO Angewandte Chemie (1983), 95(7), 552
CODEN: ANCEAD; ISSN: 0044-8249

DT Journal

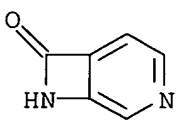
LA German

AB Naphtho[2,3-b]thiet-2-one (I) was prepared in 25% yield by flash vacuum pyrolysis of 3-mercapto-2-naphthoic acid. Methanolysis of I gave Me 3-mercapto-2-naphthoate and pyrolysis gave 2-thiocarbonyl-2H-indene. Naphtho[2,1-b]thiet-2-one was obtained quant. by pyrolysis of 1,2-dihydronaphtho[2,1-b]thiophene-1,2-dione. Naphtho[2,3-b]oxet-2-one was prepared by pyrolysis of 3-acetoxy-2-naphthoic acid or 3-hydroxy-2-naphthoyl chloride. Naphth[2,3-b]azet-2(1H)-one, azeto[3,2-b]pyridin-2(1H)-one, and azeto[2,3-c]pyridin-2(1H)-one were obtained from the corresponding aminocarboxylic acids.

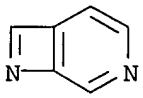
IT **86163-69-1P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 86163-69-1 CAPLUS

CN 3,8-Diazabicyclo[4.2.0]octa-1,3,5-trien-7-one (9CI) (CA INDEX NAME)



L11 ANSWER 5 OF 5 CAPLUS COPYRIGHT 2005 ACS on STN
AN 1982:561888 CAPLUS
DN 97:161888
TI Orbital topology. III. Orbital mapping of unsymmetrical molecules. A survey of the thermal ring opening of isoelectronically substituted cyclobutenes and benzocyclobutenes
AU Kelsey, Donald R.
CS Union Carbide Corp., Bound Brook, NJ, 08805, USA
SO Journal of Computational Chemistry (1982), 3(3), 436-44
CODEN: JCCHDD; ISSN: 0192-8651
DT Journal
LA English
AB Orbital mapping anal. based on CNDO/2 MO's has been used to survey the thermal ring-opening isomerizations of cyclobutenes and benzocyclobutenes. Isoelectronic substitutions within the mol. framework of cyclobutene (e.g., CH2 replaced by CH-, OH+, NH, NH2+) result in ground-state orbital correlations via both conrotatory and disrotatory pathways in several cases, in contrast to the parent hydrocarbon conrotatory stereochem. The results substantiate the heteroatom effects previously revealed by orbital mapping for the disrotatory thermal isomerizations of isoelectronic Dewar benzenes. Qual. patterns, such as nodal shifts in the butadiene π orbital, are discussed in relation to the mapping correlations. The isoelectronic benzocyclobutenes give ground-state orbital correlations via conrotatory pathways only, which suggests that delocalization may reduce the heteroatom perturbation.
IT **83352-77-6**
RL: RCT (Reactant); RACT (Reactant or reagent)
(ring cleavage of, orbital mapping anal. of)
RN 83352-77-6 CAPLUS
CN 3,8-Diazabicyclo[4.2.0]octa-1,3,5,7-tetraene (9CI) (CA INDEX NAME)



10666884

=> d his

(FILE 'HOME' ENTERED AT 19:33:48 ON 29 APR 2005)

FILE 'REGISTRY' ENTERED AT 19:33:59 ON 29 APR 2005
L1 STRUCTURE UPLOADED
L2 0 S L1
L3 3 S L1 SSS FULL

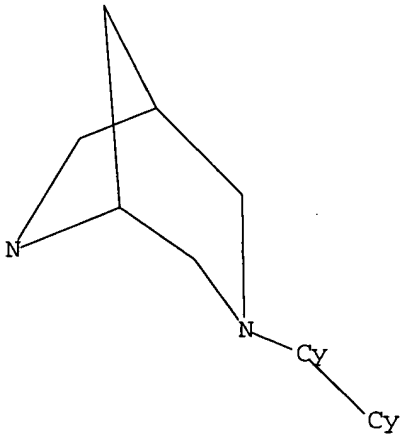
FILE 'CAPLUS' ENTERED AT 19:34:47 ON 29 APR 2005
L4 1 S L3

FILE 'MARPAT' ENTERED AT 19:35:25 ON 29 APR 2005
L5 0 S L3
L6 3 S L3 SSS FULL

FILE 'CAPLUS' ENTERED AT 19:35:49 ON 29 APR 2005
L7 3 S L6

=> s l7 not l4
L8 3 L7 NOT L4

=> d l1
L1 HAS NO ANSWERS
L1 STR



Structure attributes must be viewed using STN Express query preparation.

=> d bib abs 1-3

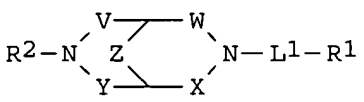
L8 ANSWER 1 OF 3 CAPLUS COPYRIGHT 2005 ACS on STN
AN 2003:950110 CAPLUS
DN **140:16752**
TI Preparation of diazabicyclic central nervous system (CNS) active agents for use in pharmaceutical compositions
IN Bunnelle, William H.; Cristina, Daniela Barlocco; Daanen, Jerome F.; Dart, Michael J.; Meyer, Michael D.; Ryther, Keith B.; Schrimpf, Michael R.; Sippy, Kevin B.; Toupence, Richard B.
PA USA

10666884

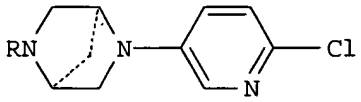
SO U.S. Pat. Appl. Publ., 49 pp., Cont. of U.S. Ser. No. 466,719.
CODEN: USXXCO
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 2003225268	A1	20031204	US 2003-412510	20030411
PRAI	US 1999-117807P	P	19990129		
	US 1999-466719	A1	19991217		

OS MARPAT 140:16752
GI



I



II

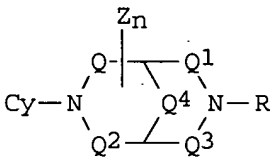
AB Diazabicyclic compds., such as I [V and X = bond or CH2; W and Y = bond, CH2, or CH2CH2; Z = CH2, CH2CH2, or CH2CH2CH2; L1 = a bond or (CH2)n; n = 1-5; R1 = heteroarom. rings, such as pyridinyl, pyrimidinyl, pyrazinyl, quinolinyl, etc.; R2 = H, alkoxycarbonyl, (amino)alkyl, aminocarbonylalkyl, benzyloxycarbonyl, cyanoalkyl, dihydro-3-pyridinylcarbonyl, hydroxy(alkyl), phenoxycarbonyl, or NH2], were prepared for therapeutic use controlling synaptic transmission in mammals. These diazabicycles are claimed for use in the treatment of Alzheimer's disease, Parkinson's disease, memory dysfunction, Tourette's syndrome, sleep disorders, attention deficit hyperactivity disorder, neurodegeneration, inflammation, neuroprotection, amyotrophic lateral sclerosis, anxiety, depression, mania, schizophrenia, anorexia and other eating disorders, AIDS-induced dementia, epilepsy, urinary incontinence, Crohn's disease, migraines, premenstrual syndrome, erectile dysfunction, substance abuse, smoking cessation, and inflammatory bowel syndrome. Thus, (1S,4S)-2-(6-chloro-3-pyridinyl)-2,5-diazabicyclo[2.2.1]heptane II (R = H) was prepared via a reaction of tert-Bu (1S,4S)-2,5-diazabicyclo[2.2.1]heptane-2-carboxylate with 2-chloro-5-iodopyridine using tert-BuONa, Pd2(dba)3 and BINAP in toluene to give the BOC-protected intermediate II (R = CO2CMe3) in 58% yield and subsequent N-deprotection of II (R = CO2CMe3) using 4N HCl/dioxane to form II (R = H) in 77% yield. The prepared diazabicycles were assayed for nicotinic acetylcholine receptor binding potency in synaptic membrane prepns. from whole rat brain and were tested for their effectiveness of nicotinic acetylcholine receptor ligands as analgesic agents in the mouse hot plate paradigm.

L8 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2005 ACS on STN
AN 2002:90615 CAPLUS
DN **136:134798**
TI Preparation of N-aryl diazabicyclic compounds for treatment of central nervous system disorders
IN Miller, Craig Harrison; Dull, Gary Maurice; Miao, Lan; Lynm, Dwo; Schmitt, Jeffrey Daniel; Clark, Thomas Jeffrey
PA Targacept, Inc., USA
SO U.S. Pat. Appl. Publ., 18 pp., Cont.-in-part of U.S. Ser. No. 578,768.
CODEN: USXXCO

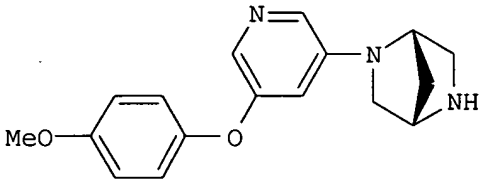
DT Patent
LA English
FAN.CNT 2

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 2002013309	A1	20020131	US 2001-864905	20010524
	US 6852721	B2	20050208		
	US 6440970	B1	20020827	US 2000-578768	20000525
	CA 2409644	AA	20011129	CA 2001-2409644	20010524
	WO 2001090109	A1	20011129	WO 2001-US16941	20010524
	WO 2001090109	C2	20030327		
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW				
	RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
	EP 1289996	A1	20030312	EP 2001-941614	20010524
	EP 1289996	B1	20050406		
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
	BR 2001010956	A	20030610	BR 2001-10956	20010524
	JP 2003534344	T2	20031118	JP 2001-586296	20010524
PRAI	US 2000-578768	A2	20000525		
	US 2001-864905	A	20010524		
	WO 2001-US16941	W	20010524		

OS MARPAT 136:134798
GI



I



II

AB The present invention relates to the preparation of N-aryl diazabicyclic compds. I [wherein Q = (CH2)u; Q1 = (CH2)v, Q2 = (CH2)w; Q3 = (CH2)x, and Q4 = (CH2)y; u, v, w, x = independently 0-4; Y = 1 or 2; Z = a non-hydrogen substituent having a sigma m value between -0.3 and about 0.75; n = 0-10; R = H or alkyl; Cy = (un)substituted Ph, pyridyl, pyrimidinyl, pyrazinyl, or 1,2,4-triazinyl] and their use in the treatment of central nervous system disorders. Of particular interest are 2-pyridyl diazabicyclic compds., such as (1S,4S)-2-(5-(3-methoxyphenoxy)-3-pyridyl)-2,5-diazabicyclo[2.2.1]heptane (II) ,(1S,4S)-2-(5-(4-methoxyphenoxy)-3-pyridyl)-2,5-diazabicyclo[2.2.1]heptane, (1S,4S)-2-(5-(3,4-dimethoxyphenoxy)-3-pyridyl)-2,5-diazabicyclo[2.2.1]heptane, (1S,4S)-2-(5-(4-fluorophenoxy)-3-pyridyl)-2,5-diazabicyclo[2.2.1]heptane, and (1S,4S)-2-(5-benzoyl-3-pyridyl)-2,5-diazabicyclo[2.2.1]heptane. The present invention also relates to prodrug derivs. of the compds. of the

present invention. For example, coupling of 3-bromo-5-(4-methoxyphenoxy)pyridine (preparation given) with (1S,4S)-N-(tert-butoxycarbonyl)-2,5-diazabicyclo[2.2.1]heptane in the presence of tris(dibenzylideneacetone)dipalladium and (rac)-2,2-bis(diphenylphosphino)-1,1-binaphthyl, and NaOBu-t in toluene, followed by deprotection using TFA and salt formation, afforded II•hemigalactarate. The latter exhibited a Ki of 13 nM in binding studies with certain CNS nicotinic receptors.

L8 ANSWER 3 OF 3 CAPLUS COPYRIGHT 2005 ACS on STN
AN 2001:868455 CAPLUS
DN **136:6011**
TI Heteroaryldiazabicycloalkanes as nicotinic cholinergic receptor ligands
IN Miller, Craig Harrison; Dull, Gary Maurice; Miao, Lan; Lynm, Dwo; Schmitt, Jeffrey Daniel; Clark, Thomas Jeffrey
PA Targacept, Inc., USA
SO PCT Int. Appl., 54 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 2

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2001090109	A1	20011129	WO 2001-US16941	20010524
	WO 2001090109	C2	20030327		
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW				
	RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
	US 6440970	B1	20020827	US 2000-578768	20000525
	CA 2409644	AA	20011129	CA 2001-2409644	20010524
	US 2002013309	A1	20020131	US 2001-864905	20010524
	US 6852721	B2	20050208		
	EP 1289996	A1	20030312	EP 2001-941614	20010524
	EP 1289996	B1	20050406		
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
	BR 2001010956	A	20030610	BR 2001-10956	20010524
	JP 2003534344	T2	20031118	JP 2001-586296	20010524
PRAI	US 2000-578768	A	20000525		
	US 2001-864905	A	20010524		
	WO 2001-US16941	W	20010524		

OS MARPAT 136:6011
AB The present invention relates to diazabicyclic compds., preferably to N-aryl diazabicyclic compds. Of particular interest are 2-pyridyl diazabicyclic compds., such as (1S,4S)-2-[5-(3-methoxyphenoxy)-3-pyridyl]-2,5-diazabicyclo[2.2.1]heptane. Other exemplary compds. of the present invention include: (1S,4S)-2-[5-(4-methoxyphenoxy)-3-pyridyl]-2,5-diazabicyclo[2.2.1]heptane (I), (1S,4S)-2-[5-(3,4-dimethoxyphenoxy)-3-pyridyl]-2,5-diazabicyclo[2.2.1]heptane, (1S,4S)-2-[5-(4-fluorophenoxy)-3-pyridyl]-2,5-diazabicyclo[2.2.1]heptane, and (1S,4S)-2-[5-benzoyl-3-pyridyl]-2,5-diazabicyclo[2.2.1]heptane. Thus, I hemigalactarate was prepared in 4 steps starting from 4-methoxyphenol and 3,5-dibromopyridine.

10666884

A binding constant of 13 nM was determined for I hemigalactarate, showing high-affinity binding to certain CNS nicotinic receptors.

RE.CNT 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

=>

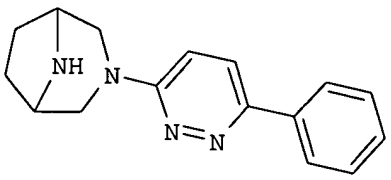
10666884

L4 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2005 ACS on STN
AN 2005:259679 CAPLUS
DN 142:336373
TI A preparation of diazabicycloakane derivatives, useful as modulators of α7 nicotinic acetylcholine receptors
IN Basha, Anwer; Bunnelle, William H.; Dart, Michael J.; Gallagher, Megan E.; Ji, Jianguo; Li, Tao; Pace, Jennifer M.; Ryther, Keith B.; Tietje, Karin R.
PA USA
SO U.S. Pat. Appl. Publ., 47 pp.
CODEN: USXXCO
DT Patent
LA English
FAN.CNT 1

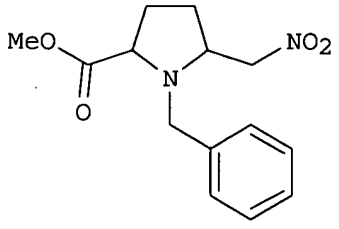
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI US 2005065178	A1	20050324	US 2003-666884	20030919
WO 2005028477	A1	20050331	WO 2004-US30735	20040917

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

PRAI US 2003-666884 A 20030919
GI



I



II

AB The invention relates to a preparation of diazabicycloakane derivs. of formula

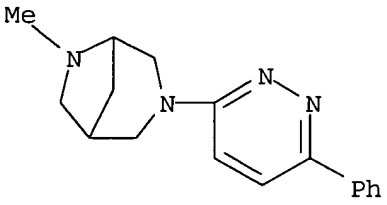
Z-Ar1-Ar2 [wherein: Z is a diazabicyclic amine; Ar1 is a 5- or 6-membered (hetero)aromatic ring; and Ar2 is selected from (un)substituted 5-membered heteroaryl ring, 6-membered heteroaryl ring, or 3,4-(methylenedioxy)phenyl, etc.], useful as modulators of α7 nicotinic acetylcholine receptors (nAChRs). The invention compds. are useful for the treatment of Alzheimer's disease, Pick's disease, AIDS dementia, and attention deficit, etc. For instance, pyridazinyldiazabicyclooctane derivative I•(p-MeC6H4SO3H)2 was prepared via heterocyclization of pyrrolidine derivative II and 7 subsequent steps (a yield of the heterocyclization step was 36%). The invention compds. had Ki values of from about 1 nM to about 10 μM.

IT **848591-71-9P**
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of diazabicycloakane derivs. useful as modulators of α7 nicotinic acetylcholine receptors)

RN 848591-71-9 CAPLUS
CN 3,6-Diazabicyclo[3.2.1]octane, 6-methyl-3-(6-phenyl-3-pyridazinyl)-, mono(4-methylbenzenesulfonate) (9CI) (CA INDEX NAME)

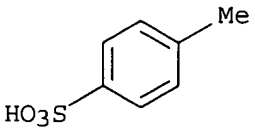
CM 1

CRN 848591-70-8
CMF C17 H20 N4



CM 2

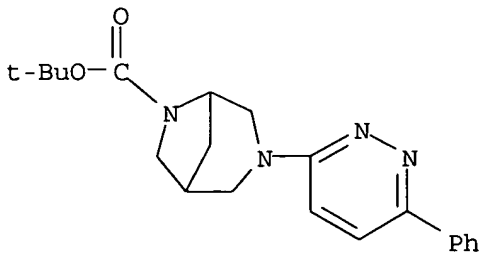
CRN 104-15-4
CMF C7 H8 O3 S



IT **848591-69-5P 848591-70-8P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of diazabicycloakane derivs. useful as modulators of α7 nicotinic acetylcholine receptors)

RN 848591-69-5 CAPLUS

CN 3,6-Diazabicyclo[3.2.1]octane-6-carboxylic acid, 3-(6-phenyl-3-pyridazinyl)-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



RN 848591-70-8 CAPLUS
CN 3,6-Diazabicyclo[3.2.1]octane, 6-methyl-3-(6-phenyl-3-pyridazinyl)- (9CI) (CA INDEX NAME)